(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization

International Bureau



. 1 (1017) 1 (1881) A CONTROL ON A CONTROL ENGINEER AND A CONTROL ON A CONTROL ON A CONTROL ON A CONTROL ON A

(43) International Publication Date 15 January 2004 (15.01.2004)

PCT

(10) International Publication Number WO 2004/004652 A2

(51) International Patent Classification7:

A61K

(21) International Application Number:

PCT/US2003/021145

(22) International Filing Date:

3 July 2003 (03.07.2003)

(25) Filing Language:

English

(26) Publication Language:

NJ 07065-0907 (US).

English

(30) Priority Data:

60/394,313

8 July 2002 (08.07.2002) US

(71) Applicant (for all designated States except US): MERCK & CO., INC. [US/US]; 126 East Lincoln Avenue, Rahway,

(72) Inventors; and

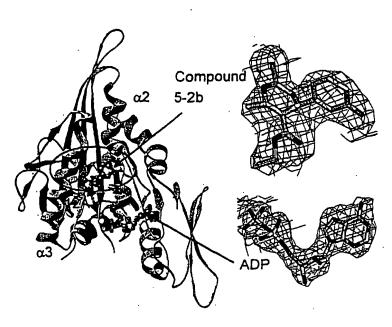
(75) Inventors/Applicants (for US only): BUSER-DOEP-NER, Carolyn, A. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). COLEMAN, Paul, J. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). COX, Christopher, D. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). FRALEY, Mark, E. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). GARBACCIO, Robert, M. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). HARTMAN, George, D. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US).

HEIMBROOK, David, C. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). KUO, Lawrence, C. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). HUBER, Hans, E. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). SARDANA, Vinod, V. [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). TORRENT, Maricel [ES/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US). YAN, Youwei [US/US]; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US).

- (74) Common Representative: MERCK & CO., INC.; 126 East Lincoln Avenue, Rahway, NJ 07065-0907 (US).
- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.
- (84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

[Continued on next page]

(54) Title: MITOTIC KINESIN BINDING SITE



(57) Abstract: The present invention is directed to the identification, characterization and three-dimensional structure of a novel ligand binding site of KSP. Binding of ligands to the novel binding site result in a conformational change in the three-dimensional structure of the protein and a modulation of the activity of KSP. This conformational change in turn results in the formation of a novel binding pocket in the KSP protein, which comprises the novel binding site of the instant invention.

WO 2004/004652 A2

WO 2004/004652 A2



Published:

without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

TITLE OF THE INVENTION MITOTIC KINESIN BINDING SITE

FIELD OF THE INVENTION

5 The present invention generally pertains to the fields of molecular biology, protein purification, protein crystallization, X-ray diffraction analysis, three-dimensional structural determination, rational drug design and molecular modeling of motor proteins, in particular -Kinesin Spindle Protein (KSP). Compositions and crystals of KSP with a 10 KSP inhibitor bound to the protein at the novel ligand binding site identified herein are also provided. The crystallized KSP is physically analyzed by Xray diffraction techniques. The resulting X-ray diffraction patterns are of sufficiently high resolution to be useful for determining the threedimensional structure of inhibitor-bound KSP. Those atomic coordinates are useful in molecular modeling of related proteins and rational drug design 15 (RDD) of mimetics and ligands for KSP and related proteins. Methods of using the structure coordinates of KSP in complex with an inhibitor for the design of pharmaceutical compositions which inhibit the biological function of KSP, particularly those biological functions mediated by molecular 20 interactions involving KSP are also disclosed.

BACKGROUND OF THE INVENTION

25

30

35

Cancer remains one of the leading causes of death in the United States. Clinically, a broad variety of medical approaches, including surgery, radiation therapy and chemotherapeutic drug therapy are currently being used in the treatment of human cancer (see the textbook CANCER: Principles & Practice of Oncology, 6th Edition, De Vita et al., eds., J. B. Lippincott Company, Philadelphia, Pa., 2001). However, it is recognized that such approaches continue to be limited by a fundamental lack of a clear understanding of the precise cellular bases of malignant transformation and neoplastic growth.

The control of cell division is one of the most basic aspects of multicellular existence. Uncontrolled cell growth and division, which produces cells that divide when they should not, produces contiguous cellular masses called tumors that are the basis for many cancers.

A common strategy for cancer therapy is the development of drugs that interrupt the cell cycle during mitosis. Compounds that perturb shortening (depolymerization) or lengthening (polymerization) cause arrest of the cell cycle in mitosis due to perturbation of the normal microtubule dynamics necessary for the chromosome movement. (Compton, D. A., et al., (1999) Science 286:913-914). A common denominator attending these compounds is that they arrest cells in mitosis by inhibiting spindle assembly (Compton, D. A., et al., (1999) Science 286:313-314). More recently, some agents such as monastrol have been implicated in inhibiting mitosis by blocking the function of essential proteins, such as mitotic proteins. (Mayer, T.U. et al., (1999) Science 286: 971-974).

5

10

15

30

35

The motor protein, kinesin, was discovered in 1985 in squid axoplasm. R. D. Vale et al., Identification of a Novel Force-generating Protein, Kinesin, Involved in Microtubule-based Motility, Cell 42:39-50 (1985). In the last few years, it has been discovered that kinesin is just one member of a very large family of motor proteins. E.g., S. A. Endow, The Emerging Kinesin Family of Microtubule Motor Proteins, 16 Trends Biochem. Sci. 221 (1991); L. S. B. Goldstein, The Kinesin Superfamily: Tails of Functional Redundancy, 1 Trends Cell Biol. 93 (1991); R. J.

Stewart et al., Identification and Partial Characterization of Six Members of the Kinesin Superfamily in Drosophila. *Proc. Nat'l Acad. Sci. USA* 88:8470 (1991). Other motor proteins include dynein, e.g. M.-G. Li et al., Drosophila Cytoplasmic Dynein, a Microtubule Motor that is Asymmetrically Localized in the Oocyte, *J. Cell Biol.* 126:1475-1493 (1994), and myosin, e.g. T. Q. P.
Uyeda et al., *J. Mol. Biol.* 214:699-710 (1990).

Mitotic kinesins are enzymes essential for assembly and function of the mitotic spindle, but are not generally part of other microtubule structures, such as in nerve processes. These essential microtubule-based motor proteins travel along microtubules reaching into every corner of the cell. Mitotic kinesins play essential roles during all phases of mitosis. These proteins can be conceptualized as biological machines that transduce chemical energy into mechanical forces and motion. Kinesins use the energy derived from ATP hydrolysis to power their movement unidirectionally along microtubules and to transport molecular cargo to specific destinations. During mitosis, kinesins organize

microtubules into the bipolar structure that is the mitotic spindle. Kinesins mediate movement of chromosomes along spindle microtubules, as well as structural changes in the mitotic spindle associated with specific phases of mitosis. Experimental perturbation of mitotic kinesin function causes malformation or dysfunction of the mitotic spindle, frequently resulting in cell cycle arrest and cell death. It is rapidly becoming clear that mictrotubule motors play a crucial role in the functions of microtubules in mitosis.

Among the mitotic kinesins which have been identified is Kinesin Spindle Protein (KSP). KSP belongs to the BimC family of 10 kinesins which are essentially a conserved kinesin subfamily of plus end-directed microtubule motors that assemble into bipolar homotetramers consisting of anti-parallel homodimers. Human KSP (also termed HsEg5) has been described [Blangy, et al., Cell, 83:1159-69 (1995); Whitehead, et al., Arthritis Rheum., 39:1635-42 (1996); Galgio et al., J. Cell Biol., 15 135:339-414 (1996); Blangy, et al., J Biol. Chem., 272:19418-24 (1997); Blangy, et al., Cell Motil Cytoskeleton, 40:174-82 (1998); Whitehead and Rattner, J. Cell Sci., 111:2551-61 (1998); Kaiser, et al., JBC 274:18925-31 (1999); GenBank accession numbers: X85137, NM004523 and U374261. and a fragment of the KSP gene (TRIP5) has been described [Lee, et al., Mol 20 Endocrinol., 9:243-54 (1995); GenBank accession number L40372]. Xenopus KSP homologs (Eg5), as well as Drosophila K-LP61 F/KRP 130 have been reported. KSP is a mitotic kinesin protein essential for proper DNA division in cells.

During mitosis KSP associates with microtubules of the mitotic spindle. Microinjection of antibodies directed against KSP into human cells prevents spindle pole separation during prometaphase, giving rise to monopolar spindles and causing mitotic arrest and induction of programmed cell death. The current model of KSP function in mitosis envisions that KSP and related kinesins in other, non-human organisms, bundle antiparallel microtubules and slide them relative to one another, thus forcing the two spindle poles apart. KSP may also mediate anaphase B spindle elongation and focussing of microtubules at the spindle pole. The mitotic spindle has been the subject of considerable research. The study of mitotic spindle proteins, such as microtubules, has yielded anti-mitotic compounds with important applications in cancer chemotherapy. The

25

30

35

demonstrated effectiveness of these anti-mitotic compounds in important medical and agricultural applications demonstrates the desirability of identifying and characterizing anti-mitotic compound development candidates.

Because defects in the function of KSP have been implicated in cell cycle arrest, agents and/or compounds that modulate the activity of this kinesin will find use in the treatment of hyper-proliferative cell disorders such as cancer.

5

10

15

20

25

30

35

Medicaments generally exhibit their biological activities through strong interactions with their respective targets. Recently, advances in protein crystallography and computational chemistry have introduced a new method of structure-based drug design into the field of drug development. X-ray crystallography (crystallography) is an established, well-studied technique that provides what can be best described as a three-dimensional picture of what a molecule looks like in a crystal. Scientists have used crystallography to solve the crystal structures for many biologically important molecules. Many classes of biomolecules can be studied by crystallography, including, but not limited to, proteins, DNA, RNA and viruses.

Crystallography has been used extensively to view ligandprotein complexes for structure-based drug design. To view such complexes, known ligands are usually soaked into the target molecule crystal, followed by crystallography of the complex. Sometimes, it is necessary to cocrystallize the ligands with the target molecule to obtain a suitable crystal.

Given a "picture" of a target biomolecule or a ligand-protein complex, scientists can look for pockets or receptors where biological activity can take place. Thereafter, scientists can experimentally or computationally design high-affinity ligands (or drugs) for the protein/receptors. Computational methods have alternatively been used to screen for the binding of small molecules. This approach is also useful for developing new anti-mitotic agents.

Recently, independent efforts have confirmed the role of mitotic kinesins as critical mediators of microtubule organization during mitosis. It is postulated that blocking the biological function of motor proteins, e.g., human KSP, will lead to cell cycle arrest. While the binary

structure of KSP complexed with ADP has been published, (Turner et al., Journal of Biological Chemistry, 276; 25496-25502 (2001), no ternary structure of KSP complexed with a modulator, e.g., inhibitor, has heretofore been published. Consequently, until the present invention, which details the structural coordinates of human KSP with various ligands, albeit inhibitors, the identity and characterization of the novel binding site detailed herein was heretofore never available for rational drug design. As such, drug discovery efforts directed towards the KSP protein have been hampered by the lack of structural information about this protein and its complex with a ligand, e.g., monastrol. Such structural information would provide valuable information in discovery of anti-mitotic agents.

5

10

15

20

25

30

The inventors provide herein crystals of KSP, complexed with a ligand, containing a novel, induced-fit binding site and have determined its three-dimensional structure. With this information, it is now possible, for the first time, to rationally design inhibitors of KSP, which can function as anti-mitotic agents, e.g. compounds which inhibit spindle pole separation during mitosis, thereby effectively inducing cell cycle arrest. It is believed that no one has heretofore reported determining the three-dimensional structure of the binding site identified herein.

Advantageous therapeutic embodiments would therefore comprise therapeutic and/or diagnostic agents based on or derived from the three-dimensional crystal structure of KSP including its novel binding site identified herein that have one or more than one of the functional activities of KSP. Additional therapeutic embodiments would comprise therapeutic and/or diagnostic agents based on or derived from molecular modeling of other members of the BimC protein family using the three-dimensional crystal structure of KSP and its binding site provided herein.

In accordance therewith, the novel-binding site disclosed herein is considered a potential target for anti-mitotic agents. In addition, the invention provides a process for creation of ligand candidate structures by means of a computer, using the structural coordinates of KSP's binding site provided herein. Furthermore, the information provided herein will enable one to search for ligand structures from a three-dimensional structure database containing known compounds.

SUMMARY OF THE INVENTION

The present invention is directed to the identification, characterization and three-dimensional structure of a novel ligand binding site of KSP. Binding of ligands to the novel binding site result in a conformational change in the three-dimensional structure of the protein and a modulation of the activity of KSP. This conformational change in turn results in the formation of a novel binding pocket in the KSP protein, which comprises the novel binding site of the instant invention. It has been further discovered that the formation of the novel binding pocket is facilitated by the concurrent binding of a nucleotide substrate or substrates to the protein. Moreover, the instant invention provides an attractive target for the rational design of potent and selective inhibitors of KSP identified by the methods of the invention, particularly new lead compounds useful in treating hyper-proliferative and KSP-dependent disorders.

15

10

5

BRIEF DESCRIPTION OF THE DRAWINGS

FIGURE 1 An X-ray oscillation diffraction picture from a crystal of KSP in complex with (+)-monastrol and ADP (Compound 5-2b).

20

25

FIGURE 2 The KSP-ADP-(+)-monastrol complex as shown in a ribbon presentation. The structure of the KSP-ADP-(+)-monastrol (Compound 5-2b) complex is shown in a ribbon representation. The bound conformations of ADP and Compound 5-2b are also given together with their respective electron density. The location of Compound 5-2b, the active isomer of monastrol, is seen at a novel induced-fit site, some 12Å distal from the nucleotide-binding site and catalytic center of the enzyme.

30

35

FIGURE 3 (+)-Monastrol binding between helix- α 2 and helix- α 3. (+)-monastrol (Compound 5-2b) is seen to bind in between (the insertion loop of) helix- α 2 and helix- α 3 (which is immediately preceding the 'Switch 1' typically seen in all kinesins). Also shown are the side-chains of Arg119, Tyr211 and Trp127. The Arg119 and Tyr211 residues move upward and outward, yielding space to accommodate the binding of the

inhibitor. At the same time, the insertion loop of helix-α2 relocates its main-chain location with a downward shift of ~8Å; the side-chain of its Trp127 as a result swings inward by ~10Å, capping the entrance of the induced-fit cavity together with the side-chains of Arg119 and Tyr211. Lining the newly formed pocket and surrounding the inhibitor are residues

5 Lining the newly formed pocket and surrounding the inhibitor are residues 115–119, 127, 130, 132–134, 136, 137, 160, 211, 214, 215, 217, 218, 221 and 239.

FIGURE 4 Comparison between the binary and ternary

structure shown in ribbon presentation. The conformational alteration observed for the kinesin structure upon Compound 5-2b binding to the ADP-binary complex is not limited to the immediate vicinity of the inhibitor. Rearrangements of protein moieties are spread throughout the enzyme upon (+)-monastrol binding, including the switch I, switch II and neck linker region, with the exception that the nucleotide binding site of the protein as well as its β-sheet structure remaining basically unchanged.

rigure 5 Conformational alteration of KSP structure upon ligand binding shown in ribbon presentation. In the Switch I area of KSP, as circled, the main-chain re-orients its geometry significantly on both ends of Ala230. Although the helicity of the Switch I region is unchanged, the pitch at the C-terminal end of helix-α3 is increased in the ternary complex from that in the binary complex.

20

25 FIGURE 6 Conformational alteration of KSP structure upon ligand binding shown in ribbon presentation. In the Switch II region of KSP, which is located on the opposite side of the binding site, as circled, the C-terminal end of helix-α-4 is repositioned significantly. The tip of the helix, in the Switch II region of KSP, near Arg305 is moved by ~6Å in the ternary complex from its location in the binary complex.

FIGURE 7 Conformational alteration of KSP structure
upon ligand binding shown in ribbon presentation. In the neck-linker region
of KSP, which is the C-terminal portion of the protein construct, the residues

beginning from Lys357 to Phe362 swing by almost 180° in the ternary complex from its position in the ADP binary complex. Although residues 363–368 are present in the protein, they are disordered in the crystal and hence offer no electron density. The neck-linker region of KSP is circled. A close-up view is depicted, comparing the neck-linker region in the ternary complex to that in the binary complex.

5

10

15

30

<u>1-368.</u>

FIGURE 8 Conformational alteration of KSP structure upon ligand binding. A close-up view comparing the nucleotide-binding site in the binary and ternary complexes of KSP is shown. Within experimental errors, most of the backbone and side-chains for the two complexes in this region of the protein can be super-positioned.

FIGURE 9 Motor Domain of Human KSP, Amino Acids

FIGURE 10 Binding Pocket of human KSP.

FIGURE 11 KSP/Compound 5-2b fluorescence data.

Compound 5-2b demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 5-2b does not cause a decrease on Trp127 fluorescence, suggesting the inability of 5-2b to bind to KSP in the absence of the nucleotide.

FIGURE 12 KSP/Compound 8-1 fluorescence data.

Compound 8-1 demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 8-1 does not cause a decrease on Trp127 fluorescence, suggesting the inability of 8-1 to bind to KSP in the absence of the nucleotide.

FIGURE 13 KSP/Compound 1-7 fluorescence data.

Compound 1-7 demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 1-7 does not cause a decrease on Trp127 fluorescence, suggesting the inability of 1-7 to bind to KSP in the absence of the nucleotide.

FIGURES 14A and 14B KSP Inhibitor Pharmacophore Models.

The two pharmacophore models derived from analysis and further computational processing of the crystallized complex are illustrated. Spheres represent a center of a hydrophobic group and boxes represent either a hydrogen bond acceptor (HA) or hydrogen bond donor (HD). All distances are in Å.

FIGURE 15 KSP Inhibitor Pharmacophore Models in KSP Binding
Site. A schematic view of the two pharmacophore models superimposed and mapped onto the ligand binding site of KSP defined, in part, by the amino acids of Figure 10.
Only relevant KSP protein residues are shown.

20 FIGURE 16 KSP Inhibitor Pharmacophore Model.

A pharmacophore model derived from analysis and further computational processing of a crystallized complex is illustrated. Spheres represent a center of a hydrophobic group and boxes represent either a hydrogen bond acceptor (HA).

25

5

TABLE 1 KSP motor domain/Compound 5-2b X-ray

TABLE 2 KSP motor domain/Compound 1-7 X-ray

30 coordinates.

coordinates.

TABLE 3 <u>KSP motor domain/Compound 2-7 X-ray</u> coordinates.

TABLE 4 KSP motor domain/Compound 4-2a X-ray

TABLE 5 Novel KSP ligand binding site/Compound 5-

5 2b X-ray coordinates.

coordinates.

10

15

20

25

30

35

DETAILED DESCRIPTION OF THE INVENTION

"Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic), and includes substitutions having an inconsequential effect on the three-dimensional structure of KSP with respect to the use of said structure for the identification and design of KSP or KSP complex inhibitors, for molecular replacement analyses and/or for homology modeling.

Amino acid sequence "similarity" is a measure of the degree to which aligned amino acid sequences possess identical amino acids or conservative amino acid substitutions at corresponding positions.

A "fragment" of KSP is meant to refer to a protein molecule which contains a portion of the complete amino acid sequence of the wild type or reference protein.

As used herein, a "variant" of a KSP protein refers to a polypeptide having an amino acid sequence with one or more amino acid substitutions, insertions, and/or deletions compared to the sequence of the invention receptor protein.

Generally, differences are limited so that the sequences of the reference (native or wild type KSP) and the variant are closely similar overall, and in many regions, identical. Such variants are generally biologically active and necessarily have less than 100% sequence identity with the polypeptide of interest.

Preferably, the biologically active variant KSP has an amino acid sequence sharing at least about 80% amino acid sequence identity with the reference KSP, preferably at least about 85%, more preferably at least about 90%, and most preferably at least about 95%. Amino-acid substitutions are preferably substitutions of single amino-acid residues. Preferably, such polypeptides also possess characteristic structural features and biological activity of a native KSP polypeptide.

For example, variants of KSP are characterized as containing key functional residues that participate in ligand binding. These polypeptide fragments, in turn, have been derivatized by methods akin to traditional drug development. Preferred polypeptides and polynucleotides of the present invention are expected to have, *inter alia*, similar biological functions/properties to their homologous polypeptides and polynucleotides. Furthermore, preferred polypeptides and polynucleotides of the present invention have at least one GPR25 activity.

Sequence similarity or percent similarity can be determined, for example, by comparing sequence information using sequence analysis software such as the GAP computer program, version 6.0, available from the University of Wisconsin Genetics Computer Group (UWGCG). The GAP program utilizes the alignment method of Needleman and Wunsch (J. Mol. Biol. 48:443, 1970), as revised by Smith and Waterman (Adv. Appl. Math. 2:482, 1981).

10

15

20

25

30

35

As used herein, a "binding site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibody or drug) via various covalent and/or non-covalent binding forces.

The terms "ligand binding site" and "binding site" are used interchangeably and refer to a region of a human KSP resulting from the complex of a ligand with KSP. It is believed that this ligand binding site, as a result of its shape and charge potential, favorably interacts or associates with a ligand or binding partner, which is preferably an inhibitor of KSP function. The binding of the ligand to this binding site induces global conformational changes to the KSP protein, thereby potentially modulating the mitotic activity of the protein and thereby inhibiting cell division and facilitating cell cycle arrest. A ligand binding site according to the present invention may include, for example, the actual site of any one of the herein disclosed compounds binding with KSP, as well as any other moiety - chemical or biological - which preferably inhibits the activities of KSP by binding to the ligand binding site disclosed herein.

As used herein, the terms "bind" and "binding" when used to describe the interaction of a ligand with a binding site or a group of amino acids means that the binding site or group of amino acids are capable of forming a covalent or non-covalent bond or bonds with the ligand.

Preferably, the binding between the ligand and the binding site or amino acid(s) is non-covalent. Such a non-covalent bond includes a hydrogen bond, an electrostatic bond, a van der Waals bond or the like. The binding of the ligand to the binding site may also be characterized by the ability of the ligand to co-crystallize with KSP within the novel binding pocket of the instant invention. It is further understood that the use of the terms "bind" and "binding" when referring to the interaction of a ligand with the novel binding site of the instant invention includes the covalent or non-covalent interactions of the ligand with all or some of the amino acid residues comprising the binding site.

5

10

15

20

25

30

A "KSP complex" refers to a co-complex of a molecule/complex comprising the KSP in bound association with a ligand either by covalent or non-covalent binding forces at the binding site disclosed herein. A non-limiting example of a KSP complex includes KSP-(+)-monastrol, or KSP bound to any one of the compounds listed herein.

The present invention relates to the three-dimensional structure of ligand bound-KSP or of a KSP analogue, and more specifically, to the structure of KSP's binding site as determined using X-ray crystallography and various computer modeling techniques. The coordinates of KSP bound to ADP and one of the ligand compounds described herein as shown in Tables 1-4 (relating to the entire motor domain), are useful for a number of applications, including, but not limited to, the characterization of a three-dimensional structure of KSP including its novel binding site, as well as the visualization, identification and characterization of a KSP ligand binding site. The ligand binding site structure(s) may then be used to predict the orientation and binding affinity of a designed or selected inhibitor of KSP, a KSP analogue or of a KSP complex. In general, KSP structures referred to herein are the KSP-ligand bound conformation of KSP. As an example, when referring to an antibody specific for the KSP of the invention, it means an antibody having an affinity for the KSP-ligand bound conformation disclosed herein.

In particular, the invention is drawn to the three-dimensional structure of a ligand bound KSP e.g., when bound to a ligand, preferably an inhibitor.

The amino acid sequence of the motor domain of human KSP is depicted in SEQ ID NO:1. These amino acids correspond to residues 1-368 of the native protein. Another aspect of the invention is a substantially pure isolated amino acid of the amino acid sequence set forth in SEQ ID NO:1. Another aspect of the invention is a variant of that isolated amino acid. Preferably the variant of the amino acid of SEQ ID NO:1 comprises one or more amino acid substitution(s) or deletion(s) of one or more of the amino acids that form the novel binding pocket of the instant invention. More preferably the variant of the amino acid of SEQ ID NO:1 comprises an amino acid substitution of one of the amino acids which form the novel binding pocket of the instant invention.

Another aspect of the invention is an isolated variant of KSP wherein the variant comprises one or more amino acid substitution(s) or deletion(s) of one or more of the amino acids that form the novel binding pocket of the instant invention. More preferably the variant of KSP comprises an amino acid substitution of one of the amino acids which form the novel binding pocket of the instant invention.

10

15

20

25

30

The KSP of the invention preferably comprises a ligand binding site characterized by the amino acid residues as set forth in Figure 10 or the relative structural coordinates of those amino acid residues according to Tables 1-4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0 Å (or more preferably, not more than about 1.0 Å, and most preferably, not more than about 0.5 Å). It is understood that the amino acids listed above represent the residues defining the novel binding pocket formed upon the complexation of a ligand of the invention with KSP. It is further understood that specific binding interactions between the listed residues may or may not occur based on the size of the ligand and structure of the ligand. It is also understood that the computational length of the allowable van der Waals interactions is also a factor when determining whether an amino acid residue binds to a ligand. It is therefore understood that the binding of a ligand of the instant invention may take place between those residues listed in Figure 10 or a subset thereof.

It has been surprisingly discovered that compounds previously disclosed as kinesin inhibitors, and other recently identified

inhibitors of KSP, bind to the KSP protein at the novel binding site described herein. In particular, (+)-monastrol (Compound 5-2b), a compound previously described as inhibiting KSP kinesin activity (see Mayer, T. U. et al. Science 286:971 (1999)) has been found to be a ligand of the novel binding site of the invention. Inhibitors of KSP have also been disclosed in pending U.S. provisional applications Ser. Nos. 60/344,453 (Case 20990PV), 60/338,383 (Case 20995PV), 60/338,380 (Case 20996PV), 60/338,779 (Case 20997PV), 60/338,344 (Case 20998PV), 60/338,379 (Case 20999PV), 60/362,922 (Case 21047PV), 60/383,449 (Case 21018PV), 60/383,478 (Case 21060PV), 60/388,621 (Case 21114PV, filed June 14, 2002) and 60/388,828 (Case 21119PV, filed June 14, 2002). Additionally, inhibitors of KSP kinesin activity are described in PCT Publications WO 01/30768 and WO 01/98278.

5

10

15

20

25

30

35

The 3-dimensional structure of KSP, bound with Mg⁺⁺-ADP and Compound 5-2b, was determined at 2.5Å resolution. Compound 5-2b was found to bind to KSP via an induced-fit some 12Å away from the catalytic center of the enzyme, resulting in the creation of a previously unknown binding pocket that is non-existent in the absence of Compound 5-2b (or the other ligands described herein). The binding of Compound 5-2b also introduced significant alteration to the structural conformation in other regions of the KSP motor protein, with the interesting exception that the nucleotide-binding pocket was virtually unaltered from that seen in the ADP binary complex. An analysis of the temperature-factor distribution in the ADP binary and ADP/5-2b ternary complexes of KSP revealed that the protein region surrounding the induced-fit binding pocket of 5-2b became highly rigid upon 5-2b binding.

Using the seeding method, high quality single crystals were obtained for KSP prepared in the presence of ADP and 5-2b. A diffraction data set to 2.5Å resolution was collected and processed in the orthorhombic P2₁2₁2₁ space group. The R_{sym} was 0.084 and the data completeness was 99%. The cell dimensions were 69.5Å, 79.5Å and 159.0Å. An oscillation X-ray diffraction picture of a KSP crystal is given in Figure 1.

The 3-dimensional, tertiary structure of KSP, bound with Mg⁺⁺-ADP and 5-2b, was determined at 2.5Å resolution with use of phases derived from a combination of molecular replacement, extensive manual

rebuilding, and dynamic refinement. Two identical protein complexes were found in the asymmetric unit of the crystal and were related by a local, non-crystallographic 2-fold axis. For each, the electron density of the protein as well as those of the ligands (ADP, Mg⁺⁺, and 5-2b) was all well defined. 5-2b was seen to be of the S handedness. Residues 2–17, 272–286, and 363–368 were disordered and showed no electron densities (The N-terminal Met1 residue was processed upon expression).

5

10

15

20

25

30

The structure of the KSP/ADP/Compound 5-2b complex is shown (Figure 2) in a ribbon representation. The bound conformations of ADP and 5-2b are also given together with their respective electron density. The location of 5-2b is seen at a novel induced-fit site, some 12Å distal from the nucleotide-binding site and catalytic center of the enzyme. An enlarged section of this region is shown in Figure 3, together with 5-2b.

In Figure 3 the Compound 5-2b is seen to bind in between (the insertion loop of) helix- α 2 and helix- α 3 (which is immediately preceding the 'Switch 1' typically seen in all kinesins). Also shown are the side-chains of Arg119, Tyr211 and Trp127. The Arg119 and Tyr211 residues move upward and outward, yielding space to accommodate the binding of the inhibitor. At the same time, the insertion loop of helix- α 2 relocates its main-chain location with a downward shift of ~8Å; the side-chain of its Trp127 as a result swings inward by ~10Å, capping the entrance of the induced-fit cavity together with the side-chains of Arg119 and Tyr211. Lining the newly formed pocket and surrounding the inhibitor are the amino acid residues listed in Figure 10. A comparison of this region in the binary and ternary complex is given in Figure 4.

The binding pocket of Compound 5-2b is novel and not previously known, insofar that this binding site does not exist until an inhibitor binds. Hence, this pocket is "induced-fit" by a ligand such as Compound 5-2b. This allosteric binding pocket, located away from the nucleotide-binding site of the motor protein, is not restricted to Compound 5-2b, but is also observed upon the crystal structure determination of complexes of KSP with other compounds of diverse chemical structure that are inhibitors of KSP activity. These results have a profound impact on the design of non-active-site directing inhibitors of KSP.

In a further embodiment of the invention is a method of causing a conformational alteration in the structure of KSP by exposing the KSP to a ligand of the novel ligand binding site of the instant invention.

The conformational alteration observed for the kinesin structure upon

Compound 5-2b binding (and the binding of other compounds) to the ADP-KSP binary complex is not limited to the immediate vicinity of the inhibitor. Rearrangements of protein moieties are spread throughout the enzyme upon 5-2b binding, with the exception that the nucleotide binding site of the protein as well as its β-sheet structure remain basically unchanged. Among the changes away from the induced-fit pocket, three are noteworthy:

1. In the Switch I area of KSP, as circled in Figure 5 and in a close-up view, the main-chain re-orients its geometry significantly on both ends of Ala230. It can be seen that although the helicity of the Switch I region is unchanged, the pitch at the C-terminal end of helix-α3 is increased in the ternary complex from that in the binary complex.

15

20

25

- 2. In the Switch II region of KSP, which is located on the opposite side of the 5-2b binding site as circled in Figure 6 and in a close-up view, the C-terminal end of helix-04 is repositioned significantly. The tip of this helix near Arg305 is moved by ~6Å in the ternary complex from its location in the binary complex.
- 3. In the neck-linker region of KSP, which is the C-terminal portion of our protein construct, the residues beginning from Lys357 to Phe362 swing by almost 180° in the ternary complex from its position in the ADP binary complex. Although residues 363–368 are present in our protein, they are disordered in the crystal and hence offer no electron density. The neck-linker region of KSP is circled in Figure 7. A close-up view is depicted comparing this region in the ternary complex to that in the binary complex.

In addition to these changes, there are other smaller regional repositionings of main-chains and side-chains of the protein. Most interestingly, the nucleotide-binding site of the motor protein, where ATP hydrolysis occurs, is basically unaltered upon 5-2b binding. A close-up view comparing this site in the binary and ternary complexes of KSP is shown in Figure 8. Within experimental errors, most of the backbone and

side-chains for the two complexes in this region of the protein can be superimposed.

The effect of overall conformational changes induced by Compound 5-2b could also be examined by comparing the distribution of temperature factors.

5

10

15

20

25

30

35

High quality single crystals were also obtained for other compounds that are inhibitors of KSP. 3-Dimensional structure determined at 2.5 Å with those crystals demonstrated that the other inhibitor compounds also induce-fit into the protein in the same manner as compound 5-2b.

Consequently, an embodiment of the invention provides protein crystals of KSP complexed with a ligand bound to the ligand binding site disclosed herein and methods for making KSP or a KSP homolog. The crystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the binding site and that interact with molecules e.g., ligands or binding partners that bind to the KSP, via the binding site.

The crystals also provide modeling information regarding the protein-ligand interaction, as well as the structure of ligands bound thereto. The KSP crystal or a KSP homolog according to the present invention can be obtained by crystallizing it with a material or compound or molecule which binds to the herein disclosed binding site of the KSP. The KSP crystal according to the present invention includes KSP (human Eg5) and the material which binds to the specific binding site of KSP.

Preferred crystalline compositions of this invention are capable of diffracting X-rays to a resolution of better than about 3.5 Å, and more preferably to a resolution of about 2.6 Å or better, and even more preferably to a resolution of about 2.0 Å or better, and are useful for determining the three-dimensional structure of the material. (The smaller the number of angstroms, the better the resolution.)

The relative structural coordinates of the amino acid residues of the KSP motor domain, when the X-ray diffraction is obtained for the crystalline complex of KSP and a ligand compound described herein, are shown in Tables 1-4.

In another aspect, the present invention provides the threedimensional structure of human KSP as well as the identification and

characterization of a binding site there within. The identification of this site permits design and identification of compounds that bind to the ligand binding site and modulate KSP related activities. The compounds include inhibitors which specifically inhibit cell proliferation.

Of equal import is the fact that knowledge of the threedimensional structure of the binding site of KSP provides a means for investigating the mechanism of action of the protein and tools for identifying inhibitors of its function.

5

10

15

20

25

30

As used herein, a ligand binding site also includes KSP or KSP analog residues which exhibit observable NMR perturbations in the presence of a binding ligand, such as any one of the herein disclosed inhibitors or any other ligand. While such residues exhibiting observable NMR perturbations may not necessarily be in direct contact with or immediately proximate to ligand binding residues, they may be critical to KSP residues for rational drug design protocols.

For example, knowledge of the three-dimensional structure of the ligand binding site allows one to design molecules, preferably pharmaceutical agents, capable of binding thereto, including molecules which are thereby capable of inhibiting the interaction of KSP with its native ligands, thereby inducing cell arrest.

Assays may be performed and the results analyzed to determine whether the agent is an inhibitor (i.e., the agent may reduce or prevent binding affinity between KSP and its native ligand/binding partner), or has no effect on the interaction between KSP and its native ligand. Agents identified using the foregoing methods, and preferably inhibitors of KSP, may then be tested as therapeutics in the treatment and/or prevention of hyper-proliferative cell disorders and other diseases that are also characterized by the presence of the hyper-proliferative cells such as cancer.

Once a KSP binding agent/inhibitor has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties – that is its affinity for the ligand binding site disclosed herein. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit the ligand binding site of KSP by the same computer methods described in detail above.

Various molecular analysis and rational drug design techniques are further disclosed in U.S. Pat. Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published as WO 99/09148, the contents of which are hereby incorporated by reference.

5

10

15

20

25

30

35

In another aspect of the instant invention, the high quality single crystals of the KSP complexes comprising the KSP, ADP and the compounds described herein could be used to obtain single crystals of a KSP complex which comprises a compound that weakly binds to KSP or one or more weakly binding fragments of a compound that binds to KSP. This method may be termed intra-crystal ligand exchange. Thus, for example and not limiting in the scope of this embodiment, high quality single crystals of KSP-ADP-Compound 5-2b complex are exposed to the crystallization buffer described in the Materials and Methods which further contains 1mM of a test compound that weakly binds to KSP. It is expected that the test compound will intercalate into the crystal and replace the compound 5-2b in the binding site. One or more molecular fragments of compounds that strongly bind to KSP may also be utilized in this technique.

X-ray diffraction data may be collected (as described in the Materials and Methods) from the high quality single crystals obtained by the intra-crystal ligand exchange technique. The 3-dimensional, tertiary structure of KSP bound to such a weakly binding compound could be utilized to guide the structural modification of the compound and, as a result, optimize the binding of the modified compound to KSP. The 3-dimensional tertiary structure of KSP bound to molecular fragment(s) could be utilized to guide in the identification of a new template for a compound having optimal binding to KSP.

Once the material is designed or selected, the affinity of the material to KSP may be calculated. For the inhibitor to be effective, it should have a high affinity for the ligand binding site, low energy difference between that energy calculated before and after binding. The affinity of the inhibitor may be measured by calculating the dissociation constant of the complex of KSP and the inhibitor. The dissociation constant is preferably 100 micromoles or less. The inhibitor preferably also maintains the bonding with KSP stably after binding. In order to do this, electrostatic repulsion such as charge-charge interactions, dipole-dipole and charge-dipole interactions between the inhibitor and KSP should not occur or be minimized. The sum of electrostatic interaction should be neutral or give a positive effect to the enthalpy of the bonding. Examples of programs designed for calculating such affinity include, but

are not limited to as follows: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. © 1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Fransisco, © 1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. © 1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif., © 1994). Using the lead compound selected by the method, a stronger inhibitor can be made or designed. This process will be described below.

5

10

15

20

25

30

35

As well, any compound or anti-mitotic agent (lead compound) selected or designed in accordance with the methods disclosed herein can be changed or modified. Atoms, substituents or a part of the structure may be altered to increase the binding affinity to KSP. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It is noted that components known in the art to alter conformation should be avoided. The substituted chemical compounds may then be analyzed for fit with KSP by the same computer methods described herein.

After the material designed by the computer method described above is prepared and bound to KSP to produce a crystal, the 3-dimensional structure of the complex may be determined at high enough resolution (over 0.28 nm) using X-ray crystallographic methods. The information gained therefrom e.g., about the interaction between KSP and the inhibitor obtained from this can then be used to modify the inhibitor and to increase the affinity of the inhibitor for the ligand binding site of KSP.

Thus, for example, those atoms considered to be involved in binding to the ligand binding site of KSP disclosed herein can be mutated by exchanging one or more of the amino acid residues in the ligand binding site or in the motor domain of KSP that eventually effects the function of KSP on the underlying cell. As an example, if a cell's hyper-proliferative state is not effected by the mutated KSP, it may be surmised that the mutation very likely has not affected the function of KSP. In the alternative scenario, where the mutation decreases the hyper-proliferative state of the diseased cell, then one may surmise that the mutation has affected the ability of KSP to function in its intended purpose, e.g. hydrolyze ATP to ADP or bind microtubule etc. due to the substitution of the amino acid residue. This method can be used to identify amino acid residues in the original KSP which are important in the binding of the ligand to the binding site of KSP disclosed herein.

Once the amino acid residues in the ligand binding site of KSP have been identified as involved in the overall function attending KSP, the structure of the binding site can be identified based on the three-dimensional structure of KSP. Based on the structure of the binding site, a compound such as a peptide or other compound can be screened and designed which will fit into the three-dimensional model of the binding site.

5

10

15

20

25

Likewise, just as the three-dimensional modeling of KSP is provided by the present invention using the coordinates from the X-ray defraction patterns, these can be either analyzed directly to provide the three-dimensional structure (if of sufficiently high resolution). Alternatively, the atomic coordinates for the crystallized KSP, as provided herein, can be used for structure determination. The X-ray diffraction patterns obtained by methods of the present invention, can be provided on computer readable media, and used to provide electron density maps.

The electron density maps, provided by analysis of the X-ray coordinates of KSP complexed with Compound 5-2b, provided herein, may then be fitted using suitable computer algorithms to generate secondary, tertiary and/or quaternary structures and/or domains of KSP, which structures and/or domains are then used to provide an overall three-dimensional structure, as well as binding and/or active sites of KSP.

Knowledge obtained concerning KSP including the binding site defined herein can also be used to model the tertiary structure of related kinesin proteins, in particular members of the BimC protein family.

As an example, the structure of renin has been modeled using the tertiary structure of endothiapepsin as a starting point for the derivation. Model building of cercarial elastase and tophozoite cysteine protease were each built from known serine and cysteine proteases that have less than 35% sequence identity. The resultant models were used to design inhibitors in the low micromolar range. (Proc. Natl. Acad. Sci. 1993, 90, 3583).

Furthermore, alternative methods of tertiary structure determination that do not rely on X-ray diffraction techniques and thus do not require crystallization of the protein, such as NMR techniques, are simplified if a model of the structure is available for refinement using the additional data gathered by the alternative technique. Thus, knowledge of the tertiary structure of the KSP binding site provides a significant window to the

structure of the other kinesin family members. Thus, an embodiment of this invention envisions use of atomic coordinates of KSP protein, or fragment, analog or variant thereof, to model a KSP protein.

5

10

15

20

25

30

One skilled in the relevant art may use conventional molecular modeling methods to identify a ligand binding site of a KSP of another species. Specifically, coordinates provided by the present invention may be used to characterize a three-dimensional structure of the target KSP molecule, liganded or unliganded. Importantly, such a skilled artisan may, from such a structure, computationally visualize a putative binding site and identify and characterize other features based upon the coordinates provided herein. Such putative ligand binding sites may be further refined using chemical shift perturbations of spectra generated from various and distinct KSP complexes, e.g. from other species, competitive and non-competitive inhibition experiments, and/or by the generation and characterization of KSP or ligand mutants to identify critical residues or characteristics of the ligand binding site.

Such identification of a putative ligand binding site is of great import in rational drug design.

It is noted that in order to use the structural coordinates generated from the complex KSP described herein in Tables 1-4, it may be necessary to display the relevant coordinates as, or convert them to, a three-dimensional shape or graphical representation, or to otherwise manipulate them. In general, such a three-dimensional representation of the structural coordinates will find use in rational drug design, molecular replacement analysis, homology modeling, and mutation analysis. This is typically accomplished using any of a wide variety of commercially available software programs capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structural coordinates. The scientific art is replete with conventional software programs, which are incorporated by reference herein in their entirety. Refer to, for example, GRID (Oxford University, Oxford, UK); AUTODOCK (Scripps Research Institute, La Jolla, Calif.); Flo99 (Thistlesoft, Morris Township, N.J.) etc.

For storing, transferring and using such programs, a machine, such as a computer, is also contemplated, which produces a three-

dimensional representation of the KSP binding site. The machine would comprise a machine-readable data storage medium comprising a data storage material encoded with machine-readable data. Machine-readable storage media comprising data storage material include conventional computer hard drives, floppy disks, DAT tape, CD-ROM, and other magnetic, magnetooptical, optical, floptical and other media which may be adapted for use with a computer. The machine further comprises a working memory for storing instructions for processing the machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machinereadable data storage medium for the purpose of processing the machinereadable data into the desired three-dimensional representation. As well, the machine of the present invention further comprises a display connected to the CPU so that the three-dimensional representation may be visualized by the user. Accordingly, when used with a machine programmed with instructions for using said data, e.g., a computer loaded with one or more programs of the sort identified above, the machine provided for herein is capable of displaying a graphical three-dimensional representation of the KSP complex described herein and set forth in Tables 1-4.

5

10

15

20

25

30

35

The structural coordinates of the present invention enable one to use various molecular design and analysis techniques in order to (i) solve the three-dimensional structures of related molecules, preferably molecular complexes such as those of other species or members of BimC family of proteins; as well as (ii) design, select, and synthesize chemical agents capable of favorably associating or interacting with a ligand binding site of a KSP molecule, wherein the molecular chemical entity would preferably inhibit KSP function including inducing mitotic arrest in cells contacted therewith.

Thus, the present invention provides a method for determining the molecular structure of a molecular complex whose structure is unknown, comprising the steps of obtaining the molecular complex whose structure is unknown, e.g., from a related species, and then generating NMR data there from. The NMR data from the molecular complex whose structure is unknown can then be compared to the structure data obtained from the KSP complex of the present invention. Then, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques can be used to conform the 3D structure described

herein for the KSP complexes disclosed in Tables 1-4 to the NMR data from unknown target molecular complex. Alternatively, molecular replacement may be used to conform the 3D structure of the present invention to X-ray diffraction data from crystals of the unknown target molecular complex.

Molecular replacement involves correctly orienting and positioning the known structure into the crystal unit cell of the unknown structure. This is accomplished by a six dimensional (three positional and three rotational) search process that involves computation of a set of theoretical diffraction data using the known structure for every orientation and position searched and comparing it with the observed diffraction data of the unknown structure. The best match defines the correct position and

5

10

15

20

25

30

35

orientation of the known structure in the unknown unit cell. This match offers phase information for use in conjunction with X-ray diffraction data of the unknown structure for the determination of its 3-dimensional structure.

In another aspect, this invention envisions use of atomic coordinates of the KSP protein disclosed herein, to design a chemical compound capable of associating with KSP or a fragment, analog or variant thereof.

For example, one method of this invention for evaluating the ability of a chemical entity to associate with any of the proteins or protein-ligand complexes set forth herein comprises the steps of: a) employing computational means to perform a fitting operation (docking) between the chemical entity and a binding pocket or other surface feature of the molecule or molecular complex; and b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

In another aspect, the invention envisions use of atomic coordinates of the KSP protein to design a model of ligands in the binding site defined herein.

Preferred embodiments of the aforementioned uses are those wherein the KSP protein comprises a binding site characterized by amino acid residues as set forth in Figure 10.

As a general rule, one may use knowledge of the geography of the various regions of the ligand binding site disclosed herein, e.g. hydrophobic and/or hydrophilic to design KSP analogs (mutant) in which

the overall KSP structure is not changed, but change does affect biological activity ("biological activity" being used here in its broadest sense to denote function). Thus, one may make changes to the amino acid sequences to effectively obtain a KSP analog/mutant that exhibits a greater affinity for its binding ligand. As well, one may correlate biological activity to structure. If the structure is not changed, and the mutation has no effect on biological activity, then the mutation has no biological function. If, however, the structure is not changed and the mutation does affect biological activity, then the residue (or atom) is essential to at least one biological function.

10

15

5

Similar molecular modeling is also provided by the present invention for rational drug design (RDD) of mimetics and ligands of KSP, "ligand" being used in the broadest sense, referring to any substance capable of observable binding to the KSP protein at the herein disclosed binding site. The drug design paradigm uses computer modeling programs to determine potential mimetics and ligands which are expected to interact with sites on the protein. The potential mimetics or ligands are then screened for activity and/or binding. For KSP-related mimetics or ligands, screening methods can be selected from assays for at least one biological activity of KSP, e.g., antimitotic activity. Thus, an embodiment of the invention envisions use of the structural information from the ligand/protein complexes found herein including the information derived therefrom in designing new chemical or biological moieties that bind tighter, bind more specifically, have better biological activity or have better safety profile than known ligands that bind KSP.

25

30

20

The computer modeling method disclosed herein can also be used to remodel the mimetics or ligands to improve the affinity or solubility, and produce an optimized pharmaceutical agent.

The resulting optimized mimetics or ligands can thereafter be prepared and the inhibitory activity for KSP can be tested *in vitro* and *in vivo*. If the test confirms that the material does indeed inhibit KSP, then the material or a derivative can be used as an anti-mitotic agent. Using the method as described above, the compound identified to have inhibitory activity may thereafter be used as a lead compound to obtain an improved inhibitor.

In order to confirm the affinity predicted by the computer modeling method, the dissociation constant of the complex may be experimentally measured.

The resulting mimetics or ligands are then provided by methods of the present invention and are useful for treating, inhibiting or preventing KSP-modulated diseases in animals, including humans.

Preferably the ligands of the novel binding site provided herein are useful in the treatment or prevention of a hyper-proliferative disease, preferably cancer. Preferably, the ligand(s) identified by the methods described herein are useful in the treatment of cancer.

5

10

15

20 -

25

30

The ligands identified by the methods of this invention may be administered to mammals, preferably humans, either alone or, preferably, in combination with pharmaceutically acceptable carriers, excipients or diluents, in a pharmaceutical composition, according to standard pharmaceutical practice. The ligands can be administered orally or parenterally, including the intravenous, intramuscular, intraperitoneal, subcutaneous, rectal and topical routes of administration.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specific amounts, as well as any product which results, directly or indirectly, from combination of the specific ingredients in the specified amounts.

The pharmaceutical compositions containing the active ingredient may be in a form suitable for oral use, for example, as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules, emulsions, hard or soft capsules, or syrups or elixirs. When a ligand according to this invention is administered into a human subject, the daily dosage will normally be determined by the prescribing physician with the dosage generally varying according to the age, weight, sex and response of the individual patient, as well as the severity of the patient's symptoms.

In one exemplary application, a suitable amount of a ligand of the novel KSP ligand binding site is administered to a mammal undergoing treatment for cancer. Administration occurs in an amount between about 0.1 mg/kg of body weight to about 60 mg/kg of body weight per day, preferably of between 0.5 mg/kg of body weight to about 40 mg/kg of body weight per day.

Consequently, an object of the invention is to provide a method for determining the three-dimensional structure of a protein containing the ligand binding site as disclosed herein, or a complex of the protein with a ligand thereof, using homology modeling techniques and structural coordinates for a composition of this invention. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related proteins, protein domains and/or subdomains. Homology modeling may be conducted by fitting common or homologous portions of the protein or peptide whose three-dimensional structure is to be solved to the three-dimensional structure of homologous structural elements. Homology modeling can include rebuilding part or all of a three-dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved.

5

10

35

One of the objects of this invention is to provide three-15 dimensional structural information on new complexes of BimC family members of which KSP is a member with various ligands, as well as muteins or other variants of any of the foregoing. To that end, the invention provides for the use of the structural coordinates of a crystalline composition of this invention, or portions thereof, to solve, e.g., by 20 molecular replacement, the three-dimensional structure of a crystalline form of such a ligand-protein complex, typically involving a protein containing at least one ligand binding site as disclosed herein. Doing so involves obtaining X-ray diffraction data for crystals of the protein-ligand complex for which one wishes to determine the three-dimensional structure. Then, 25 one determines the three-dimensional structure of that protein or complex by analyzing the X-ray diffraction data using molecular replacement techniques with reference to the previous structural coordinates. As described in U.S. Pat. No. 5,353,236, for instance, molecular replacement uses a molecule having a known structure as a starting point to model the structure of an 30 unknown crystalline sample.

Still further, the invention also includes compositions and methods for identifying binding sites of other members of the BimC protein family. The methods involve examining the surface of a protein of interest, preferably a kinesin, to identify residues that facilitate binding to the binding site. The residues can be identified by homology to the ligand binding site of

human KSP described herein. Overlays and super-positioning with a threedimensional model of a KSP binding site, or a portion thereof that contains a ligand binding site, also can be used for this purpose.

An alternative method of this invention provides for selecting from a database of chemical structures a compound capable of binding to a BimC family protein. The method starts with structural coordinates of a crystalline composition of the invention, e.g., coordinates defining the three-dimensional structure of a BimC family protein or a portion thereof e.g., the herein provided coordinates relative to human KSP.

5

10

15

20

25

30

35

Points associated with that three-dimensional structure are characterized with respect to the extent of favorable interactions with one or more functional groups. A database of chemical structures is then searched for candidate compounds containing one or more functional groups disposed for favorable interaction with the protein based on the prior characterization.

Compounds having structures which best fit the points of favorable interaction with the three-dimensional structure are thus identified.

An exemplary embodiment of the invention provides methods for identifying and designing small molecules that bind to the binding site using atomic models of KSP provided herein. The method involves modeling test compounds that fit spacially into the binding site of interest using an atomic structural model comprising a KSP binding site or portion thereof, screening the test compounds in a biological assay characterized by binding of a test compound to KSP, and identifying a test compound that binds to KSP.

Also provided is a method for identifying a potential inhibitor of KSP, comprising the steps of using a three-dimensional structure of a KSP binding site as defined by the relative structural coordinates set forth in Table 5 or the relative structural coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 to design or select a potential inhibitor, and obtaining or synthesizing said potential inhibitor. The inhibitor may be selected by screening an appropriate database, may be designed de novo by analyzing the steric configurations and charge potentials of an empty KSP binding site in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors to create "hybrid" inhibitors. The inhibitor may then be contacted with KSP, and the effect of

the inhibitor on KSP related function may be assessed. For instance, a potential inhibitor identified by this method may be contacted with KSP in the presence of one or two KSP substrates selected from ATP and microtubules, and determining the effect the potential inhibitor has on KSP ATPase activity. It is also within the confines of the present invention that a potential inhibitor may be designed or selected by identifying chemical entities or fragments capable of associating with KSP; and assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential inhibitor.

In furtherance of the above, there is provided a method for identifying an anti-mitotic agent comprising providing the atomic coordinates comprising the relative atomic structural coordinates of the amino acids of Figure 10 as set forth in Tables $1-4\pm a$ root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.00Å thereof to a computerized modeling system; modeling compounds which fit spacially into the KSP binding site; and identifying in an assay for KSP activity a compound that inhibits or decreases the activity of the KSP through binding to the binding site.

Once the agent has been identified, it may be contacted with KSP and the effect the agent has on KSP may then be assessed. In addition, the agent may be contacted with KSP in the presence of a KSP binding molecule and the effect the agent has on binding between KSP and the KSP binding molecule may then be assessed.

Also disclosed herein is a process for identifying a potential anti-mitotic agent which upon binding to a human KSP inhibits cell proliferation, the process comprising the steps of:

- exposing the KSP to a mixture of at least two potential ligands;
- b) attempting to crystallize said KSP in the presence of said mixture;
- c) if crystals are obtained, obtaining an X-ray diffraction pattern of the KSP crystal; and
- d) determining whether a ligand/KSP complex is formed by comparing the electron density map calculated from the X-ray diffraction pattern of said KSP crystal

35

5

10

15

20

25

30

when exposed to said mixture of said at least two potential ligands to the electron density map calculated from the X-ray diffraction pattern set forth in a table selected from Table 1, 2, 3 and 4.

Also provided herein is a method of identifying a compound that modulates the binding of a ligand to a ligand binding site of a human KSP, said method comprising: modeling test compounds that fit spatially into a KSP ligand binding site using an atomic structural model of a KSP binding site having the relative structural coordinates as set forth in a table selected from the group consisting of Tables 1, 2, 3 and 4 for the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; screening the test compounds in an assay characterized by binding of a ligand to the ligand binding site; and identifying a test compound that modulates binding of said ligand to the KSP at its binding site.

5

10

15

20

30

35

Further provided is a method for identifying a potential inhibitor of human kinesin spindle protein (KSP), the method comprising the steps of:

- (i) providing a three-dimensional structure of a ligandbound KSP as defined by atomic coordinates set forth in a table selected from Tables 1, 2, 3 and 4;
- (ii) comparing the three-dimensional coordinates of the ligand when it is bound to KSP as set forth in Table 1, 2, 3 or 4 to the threedimensional coordinates of a compound in a database of compound structures; and
 - (iii) selecting from said database at least one compound that is structurally similar to said ligand when it is bound to said KSP, wherein the selected compound is a potential inhibitor of said KSP.

Also provided is a method for identifying an anti-mitotic agent which upon binding to a target human KSP inhibits cell proliferation, the method comprising the steps of:

a) exposing a target KSP to a mixture of at least two potential ligands;

 attempting to crystallize said target KSP in the presence of said mixture;

- c) obtaining a crystal of said target KSP exposed to said mixture to determine whether ligand/KSP complex is formed; and
- d) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.

5

15

25

30

Further provided is a method for identifying an anti-mitotic
agent which upon binding to a target human KSP inhibits cell proliferation,
the method comprising the steps of:

- (a) obtaining a crystal of KSP, where said KSP has been crystallized while exposed to a mixture of at least two potential ligands;
- (b) determining whether a ligand/KSP complex is formed in said crystal; and
- (c) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.
- In the methods described hereinabove, potential ligands of KSP include the test compounds and Mg++ and ADP.

Also provided is a method of modulating, e.g., inhibiting the activity of a KSP. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the binding site disclosed herein.

Also provided is a method of identifying a compound that selectively inhibits the activity of one type of KSP compared to other KSPs or kinesins, e.g., a KSP of one species over another or a KSP over another member of the BimC family, of which KSP is a member. Thus, the method enables the identification of KSP and KSP like proteins in the same family, e.g., BimC or the KSP in one species over another. The method is exemplified by modeling test compounds that fit spacially and preferentially into a KSP ligand binding site of interest using an atomic structural model of

a KSP ligand binding site, selecting a compound that interacts with one or more residues of the ligand binding site unique in the context of that site, and identifying in an assay for ligand binding activity a compound that selectively binds to the ligand binding site compared to other KSP. The unique features involved in receptor-selective ligand binding can be identified by comparing atomic models of different receptors or isoforms of the same type of receptor.

5

10

15

20

25

30

35

The present invention also provides for computer programs for the expression (such as visual display) of the KSP or analog three-dimensional structure, and further, a computer program which expresses the identity of each constituent of a KSP molecule and the precise location within the overall structure of that constituent, down to the atomic level.

There are many currently available computer programs for the expression of the three-dimensional structure of a molecule. Generally, these programs provide for inputting of the coordinates for the three-dimensional structure of a molecule (i.e., for example, a numerical assignment for each atom of a KSP molecule along an x, y, and z axis or the assignment for each atom of the binding site described in Tables 1-4), means to express (such as visually display) such coordinates, means to alter such coordinates and means to express an image of a molecule having such altered coordinates. One may program crystallographic information, i.e., the coordinates of the location of the atoms of a KSP binding site molecule in three dimension space, wherein such coordinates have been obtained from crystallographic analysis of said KSP molecule, into such programs to generate a computer program for the expression (such as visual display) of the KSP three-dimensional structure.

In furtherance of the above, the present invention provides a machine, such as a computer, programmed in memory with the coordinates of KSP or portions thereof, together with a program capable of converting the coordinates into a three-dimensional graphical representation of the structural coordinates on a display connected to the machine.

As well, there is provided a computer program for the expression of KSP's three-dimensional structure together with the structure of the novel KSP binding site. Preferred is the computer program QUANTA 2000, available from Molecular simulations or Insight II, version 4, available

from Biosym, San Diego, Calif., with the coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 input. Preferred expression means are well known to a skilled artisan. Alternatively, the present KSP crystallographic coordinates and diffraction data are also deposited in the Protein Data Bank, Chemistry Department, Brookhaven National Laboratory, Upton, N.Y. 119723, USA. One may use these data in preparing a different computer program for expression of the three-dimensional structure of a KSP molecule or analog thereof.

5

10

15

20

25

30

35

Structural coordinates of a crystalline composition of this invention may be stored in a machine-readable form on a machine-readable storage medium, e.g. a computer hard drive, diskette, DAT tape, etc., for display as a three-dimensional shape or for other uses involving computer-assisted manipulation of, or computation based on, the structural coordinates or the three-dimensional structures they define. For example, data defining the three-dimensional structure of a KSP protein or portions or structurally similar homologues of such proteins, may be stored in a machine-readable storage medium, and may be displayed as a graphical three-dimensional representation of the protein structure, typically using a computer capable of reading the data from said storage medium and programmed with instructions for creating the representation from such data.

This invention thus encompasses a machine, such as a computer, having a memory which contains data representing the structural coordinates of a crystalline composition of this invention, e.g. the coordinates set forth in Tables 1-4, together with additional optional data and instructions for manipulating such data. Such data may be used for a variety of purposes, such as the elucidation of other related structures and drug discovery. For example, a machine having a memory containing such data aids in the rational design or selection of inhibitors of KSP binding or activity, including the evaluation of the ability of a particular chemical entity to favorably associate with KSP as disclosed herein, as well as in the modeling of compounds, proteins, complexes, etc. related by structural or sequence homology to KSP.

Thus, three-dimensional modeling of KSP provided by the present invention using the coordinates from the X-ray diffraction patterns can be entered into one or more computer programs for molecular modeling.

Such molecular modeling programs generate atomic coordinates that reflect the secondary, tertiary and/or quaternary structures of the protein which contribute to its overall three-dimensional structure and provide information related to binding and/or active sites of the protein.

5

10

15

20

25

30

35

The present invention further contemplates the use of the structural coordinates of the present invention with standard homology modeling techniques to determine the unknown three-dimensional structure of a target molecule or molecular complex. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related protein molecules/molecular complexes or parts thereof (i.e., ligand binding sites). In general, homology modeling entails fitting common or homologous portions of the protein whose three-dimensional structure is to be solved to the three-dimensional structure of homologous structural elements in the known molecule, specifically using the relevant (i.e., homologous) structural coordinates provided in Tables 1-4. Homology may be determined using amino acid sequence identity, homologous secondary structure elements, and/or homologous tertiary folds. Homology modeling can include rebuilding part or all of a three-dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved. Examples of programs for homology modeling include, but are not limited to: QUANTA (Molecular Simulations, Inc.), Molecular Operating Environment or MOE (Chemical Computing Group, Inc. 2002), MODELLER (copyright @ 1989-2002 Andrej Sali; Departments of Biopharmaceutical Sciences and Pharmaceutical Chemistry, and California Institute for Quantitative Biomedical Research, Mission Bay Genentech Hall, University of California San Francisco) and others.

In accordance with the above, a three-dimensional structure for the unknown molecule/molecular complex may be generated using the three-dimensional structure of the KSP molecule of the present invention, Tables 1-4, refined using a number of techniques well known in the art, and then used in the same fashion as the structural coordinates of the present invention, for instance, in applications involving molecular replacement analysis, homology modeling, and rational drug design.

Among other aspects, the coordinates in Table 1-4 define the relative relationship between the protein, the nucleotide and the ligand. Such sets of

coordinates are dependent upon the particular coordinate system used. Those skilled in the art will recognize that rotation, translation or other mathematical manipulation of these coordinates may change the specific values of these coordinates, but the new set(s) will still define the relationship between the multiple components of the crystal structure disclosed herein."

5

10

15

20

25

30

35

The determination of the three-dimensional structure of the ligand binding site of KSP as disclosed herein is advantageous over conventional drug assay techniques, in which the only way to identify such an agent is to screen thousands of test compounds until an agent having the desired inhibitory effect on a target compound is identified. Generally, such conventional screening methods are expensive, time consuming, and do not elucidate the method of action of the identified agent on the target compound. In sharp contrast, advancing X-ray, spectroscopic and computer modeling technologies allow researchers to visualize the three-dimensional structure of a targeted compound (i.e., KSP ligand binding site), and using such a three-dimensional structure to identify putative binding sites and then identify or design agents to interact with these binding sites. These agents can thereafter be screened for an inhibitory effect upon the target molecule. Consequently, an embodiment of the invention details a method for identifying a potential inhibitor of KSP. The proposed method comprises using a three-dimensional structure of KSP and the novel binding site of the invention as defined by the relative structural coordinates of Tables 1-4 and the relative structural coordinates of the amino acid residues of Figure 10 as set forth in Table 1-4 to design or select a potential inhibitor of KSP activity. followed by synthesizing or obtaining the said potential inhibitor. The inhibitor may be selected by screening an appropriate database. Alternatively, it may be designed de novo by analyzing the steric configurations and charge potentials of a ligand bound KSP complex in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors of KSP.

An entity/agent that interacts or associates with the ligand binding site of KSP may be identified by performing computer fitting analyses to identify an agent which interacts or associates with said site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the binding site and the identified agent, by (a)

generating a three-dimensional model of the ligand binding site using homology modeling or the atomic structural coordinates of the binding site in Tables 1-4, and (b) determining the degree of association between the binding site and the identified agent. The degree of association may be determined computationally by any number of commercially available software programs, or may be determined experimentally using standard binding assays.

5

10

15

20

25

30

35

Preferably, the method of the present invention includes the use of a ligand binding site characterized by the three-dimensional structure comprising the relative structural coordinates of amino acid residues listed in Figure 10 as set forth in Tables $1-4\pm a$ root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0~Å, preferably not more than about 1.0~Å, and most preferably not more than about 0.5~Å. It is understood that the method of the present invention includes additional embodiments comprising conservative substitutions of the noted amino acids which result in the same structural coordinates of the corresponding residues in Tables 1-4 within the stated root mean square deviation.

The effect of an agent identified by computer fitting analyses on human KSP activity may be further evaluated computationally, or experimentally by competitive binding experiments or by contacting the identified agent with KSP and measuring the effect of the agent on the target's biological activity. Standard enzymatic assays may be performed and the results analyzed to determine whether the agent is an inhibitor of KSP activity (i.e., induce cell cycle arrest or inhibit the association of KSP with a microtubule as well as any other known activities attending a kinesin). Further tests may be performed to evaluate the selectivity of the identified agent to KSP with regard to other KSP proteins (other species) or other members of the BimC protein family.

Preferably, the agent designed or selected to interact with KSP is capable of associating with KSP and of assuming a three-dimensional configuration and orientation that complements the relevant ligand binding site of KSP.

Consequently, using these criteria, the structural coordinates of the KSP molecule as disclosed herein, and/or structural coordinates

derived therefrom using molecular replacement or homology modeling, agents may be designed having increased potency and/or selectivity versus known inhibitors, e.g, by modifying the structure of known inhibitors or by designing new agents de novo via computational inspection of the three-dimensional configuration of KSP's novel ligand binding site described herein (relative structural coordinates of amino acid residues listed in Figure 10 as set forth in Tables 1-4 and the relative structural coordinates set forth in Table 5).

5

10

15

20

25

30

35

As such, an embodiment of the invention proposes using the structural coordinates of Tables 1-4 of the present invention, or structural coordinates derived therefrom using molecular replacement or homology modeling techniques as discussed above to screen a database for agents that may act as potential inhibitors of KSP activity. As an example, the obtained structural coordinates of the present invention may be read into a software package and the three-dimensional structure analyzed graphically. A number of computational software packages may be used for the analysis of structural coordinates, e.g., Sybyl (Tripos Associates) etc. Additional software programs may be optionally used to check the coordinates with regard to features such as bond and atom types. If necessary, the threedimensional structure may be modified and then energy minimized using the appropriate software until all of the structural parameters are at their equilibrium/optimal values. The energy minimized structure can then be superimposed against the original structure to make sure there are no significant deviations between the original and the energy minimized coordinates.

Once the specific interaction between KSP and a known inhibitor is determined, e.g., such as the information provided in Tables 1-4, docking studies with different inhibitors will allow one skilled in the art to generate initial models of new inhibitors bound to KSP. The integrity of these new models may be evaluated a number of ways, including constrained conformational analysis using molecular dynamics methods; that is where both KSP and the bound inhibitor are allowed to sample different three-dimensional conformational states until the most favorable state is reached or found to exist between the protein and the bound agent etc. Once models are obtained of the original known agent bound to KSP

(Tables 1-4) and computer models of other molecules bound to KSP are as well obtained, strategies may be proposed determined for designing modifications into the inhibitors to improve their activity and/or enhance their selectivity.

5

10

15

25

30

35

For example, once a KSP binding agent has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties for KSP. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit to KSP by the same computer methods described in detail above. Further molecular analysis and rational drug design techniques are disclosed in U.S. Pat. Nos. 5,834,228, and 5,939,528 the contents of which are incorporated by reference in their entirety.

Thus, an exemplary embodiment of the invention envisions a method of three-dimensional modeling of a KSP protein, comprising the steps of:

- (a) providing three-dimensional atomic coordinates derived from
 X-ray diffraction measurements of a KSP protein in a computer readable format;
 - (b) inputting the data from step (a) into a computer with appropriate software programs; and
 - (c) generating a three-dimensional structural representation of the KSP protein suitable for visualization and further computational manipulation.

This invention further provides for the use of the structural coordinates of a crystalline composition of this invention, or portions thereof, to identify reactive amino acids within the three-dimensional structure, preferably within or adjacent to a ligand binding site; to generate and visualize a molecular surface, such as a water-accessible surface or a surface comprising the space-filling van der Waals surface of all atoms; to calculate and visualize the size and shape of surface features of the protein or complex, e.g., ligand binding pockets; to locate potential H-bond donors and acceptors within the three-dimensional structure, preferably within or

adjacent to a ligand binding site; to calculate regions of hydrophobicity and hydrophilicity within the three-dimensional structure, preferably within or adjacent to a ligand binding site; and to calculate and visualize regions on or adjacent to the protein surface of favorable interaction energies with respect to selected functional groups of interest (e.g. amino, hydroxyl, carboxyl, methylene, alkyl, alkenyl, aromatic carbon, aromatic rings, heteroaromatic rings, substituted and unsubstituted phosphates, substituted and unsubstituted phosphonates, substituted and unsubstituted fluoro and difluorophosphonates; etc.). One may use the foregoing approaches for characterizing the protein and its interactions with moieties of potential ligands to design or select compounds capable of specific covalent attachment to reactive amino acids (e.g., cysteine) and to design or select compounds of complementary characteristics (e.g., size, shape, charge, hydrophobicity/hydrophilicity, ability to participate in hydrogen bonding, etc.) to surface features of the protein, a set of which may be preselected. Using the structural coordinates, one may also predict or calculate the orientation, binding constant or relative affinity of a given ligand to the protein in the complexed state, and use that information to design or select compounds of improved affinity.

5

10

15

20

25

30

35

In such cases, the structural coordinates of the KSP protein, or portion or complex thereof, are entered in machine readable form into a machine programmed with instructions for carrying out the desired operation and containing any necessary additional data, e.g. data defining structural and/or functional characteristics of a potential ligand or moiety thereof, defining molecular characteristics of the various amino acids, etc.

The present invention is additionally directed to a method of determining the three-dimensional structure of a molecule or molecular complex whose structure is unknown, comprising the steps of first obtaining crystals of the molecule or molecular complex whose structure is unknown, and then generating X-ray diffraction data from the crystallized molecule or molecular complex and/or generating NMR data from the solution of the molecule or molecular complex. The generated diffraction or spectroscopy data from the molecule or molecular complex can then be compared with the solution coordinates or three-dimensional structure of KSP as disclosed herein, and the three-dimensional structure of the unknown molecule or

molecular complex conformed to the KSP structure using standard techniques such as molecular replacement analysis, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques, and computer homology modeling. Alternatively, a three-dimensional model of the unknown molecule may be generated by generating a sequence alignment between KSP and the unknown molecule, based on any or all of amino acid sequence identity, secondary structure elements or tertiary folds, and then generating by computer modeling a three-dimensional structure for the molecule using the three-dimensional structure of, and sequence alignment with, KSP.

5

10

15

20

25

30

Preferred embodiments of the aforementioned methods are those methods wherein the KSP protein comprises a binding site characterized by amino acid residues described in Figure 10.

This invention also provides peptidomimetic methods for designing a compound capable of binding to a KSP protein or KSP homolog. One such method involves graphically displaying a three-dimensional representation based on coordinates defining the three-dimensional structure of a KSP family protein or a portion thereof complexed with a ligand. Interactions between portions of a ligand and the protein may then be analyzed in order to identify candidate moieties for replacement. One or more portions of the ligand which interact with the protein may be replaced with substitute moieties selected from a knowledge base of one or more candidate substitute moieties, and/or moieties may be added to the ligand to permit additional interactions with the protein.

In another aspect of the instant invention, the structural coordinates of a crystalline composition of this invention, or portions thereof, may be used to identify one or more pharmacophores of a chemical compound that binds to the ligand binding site. Such a pharmacophore is described as a set of atoms, chemical groups, pseudo-atoms or vectors, and the relative positions in space of each of these pharmacophore features. Each feature, alone or in combination with its relative position, forms a pharmacophore parameter. Thus, the pharmacophore includes the pharmacophore features, and the relative position of each descriptor with regard to all other descriptors comprising the pharmacophore.

Pharmacophore models can be constructed either directly or indirectly.

In the direct method, the pharmacophore feature spatial centers are inferred from

studying the X-ray structural coordinates or NMR structure of a receptor-ligand complex, followed by a shape-complementarity function analysis of the receptor binding site, usually performed using a computer and a computer-readable medium. In the indirect method, the structure of the receptor is unknown and the pharmacophore feature spatial centers are inferred by overlaying the three-dimensional conformations of active compounds and finding the common, overlapping functional groups.

5

10

15

20

25

30

35

The pharmacophore models of the present invention, obtained by combining both direct and indirect methods, are herein described, by way of example only and without any intention of being limiting, with reference to Figures 14A and B.

The first model pharmacophore (FIG. 14A) is represented by three pharmacophore features having the planar orientation shown: a sphere indicating the center of an aryl, heteroaryl or cycloalkyl ring (or, in general, of a hydrophobic group), and two small boxes (labeled HA and HD), representing the heterocenters of a hydrogen bond acceptor and a hydrogen bond donor, respectively. The second model pharmacophore (FIG. 14B) is represented by three pharmacophore features: two spheres indicating the centers of two aryl, heteroaryl or cycloalkyl rings (or hydrophobic groups in general), and a small box representing the heteroatomic center of a hydrogen bond acceptor (HA).

As used herein, "aryl" is intended to mean any stable monocyclic or bicyclic carbon ring of up to 7 atoms in each ring, wherein at least one ring is aromatic. Examples of such aryl elements include phenyl, naphthyl, tetrahydronaphthyl, indanyl and biphenyl. In cases where the aryl substituent is bicyclic and one ring is non-aromatic, it is understood that attachment is via the aromatic ring.

The term heteroaryl, as used herein, represents a stable monocyclic or bicyclic ring of up to 7 atoms in each ring, wherein at least one ring is aromatic and contains from 1 to 4 heteroatoms selected from the group consisting of O, N and S. Heteroaryl groups within the scope of this definition include but are not limited to: acridinyl, carbazolyl, cinnolinyl, quinoxalinyl, pyrrazolyl, indolyl, benzotriazolyl, furanyl, thienyl, benzothienyl, benzofuranyl, quinolinyl, isoquinolinyl, oxazolyl, isoxazolyl, indolyl, pyrazinyl, pyridazinyl, pyridinyl, pyrimidinyl, pyrrolyl, tetrahydroquinoline. In an embodiment of the instant invention, heteroaryl does not include quinazolinone.

As used herein, "cycloalkyl" is intended to include monocyclic saturated aliphatic hydrocarbon groups having the specified number of carbon atoms.

For example, "cycloalkyl" includes cyclopropyl, methyl-cyclopropyl, 2,2-dimethyl-cyclobutyl, 2-ethyl-cyclopentyl, cyclohexyl, and so on. In an embodiment of the invention the term "cycloalkyl" includes the groups described immediately above and further includes monocyclic unsaturated aliphatic hydrocarbon groups. For example, "cycloalkyl" as defined in this embodiment includes cyclopropyl, methyl-cyclopropyl, 2,2-dimethyl-cyclobutyl, 2-ethyl-cyclopentyl, cyclohexyl, cyclopentenyl, cyclobutenyl and so on.

5

10

15

20

25

30

35

The, cycloalkyl, aryl, heteroaryl and heteroaryl substituents may be substituted or unsubstituted, unless specifically defined otherwise. For example, an aryl may be substituted with one, two or three substituents selected from OH, alkyl, halogen, alkoxy or dialkylamino.

The active structural motifs designated herein as the model pharmacophores of the present invention can be used to screen libraries of molecules for the existence of a predefined structural motif, and in particular identifying molecules that meet the constraints imposed by the pharmacophore. The pharmacophore feature spatial centers are globally associated with a specific biological activity. The molecules being evaluated may be designed *de novo* using computer methods, or alternatively, be either a scaffold or a full chemical entity (e.g., chosen from a library of compounds). Using the model pharmacophores disclosed herein one of ordinary skill may predict the inhibitory potency of a compound based upon its fit with any of these two pharmacophore models shown in FIG. 14A and B.

In an embodiment, the compound identified by the use of a pharmacophore model described herein has a binding affinity for KSP of about 0.1 nM to about 100 nM. In a further embodiment, the binding affinity range is from about 1 nM to about 20 nM.

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 14A does not incorporate a 2-thioxo-1,2,3,4-tetrahydropyrimidine moiety, a dihydropyrimidine moiety or a 5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]-pyrido[3.4-b]indole-1,3(2H)-dione moiety.

An additional pharmacophore model is illustrated by Figure 16. The pharmacophore model of Figure 16 is represented by four pharmacophore features: three spheres indicating the centers of aryl, heteroaryl or cycloalkyl rings (or hydrophobic groups in general), and a small box representing the heteroatomic center of a hydrogen bond acceptor (HA). In reference to Figure 16, the distances in Å between the pharmacophore features are listed in the following table:

	1	2	3	4
1	-			
. 2	5.1±0.6	-		
3	8.5±0.7	6.9±0.7	-	
4	3.7±0.5	5.8±0.6	5.7±0.7	-

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 16 does not incorporate a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety. In a further embodiment, the compound identified by its fit with the pharmacophore model of Figure 16 does not incorporate a quinazolinone, phenothiazine or triphenylmethane moiety.

5

10

15

20

25

30

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 14B does not incorporate a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety. In a further embodiment, the compound identified by its fit with the pharmacophore model of Fig. 14B does not incorporate a quinazolinone, phenothiazine or triphenylmethane moiety.

The degree of fit of a particular compound structure to the pharmacophore models is calculated by determining, using computer methods, if the compound possesses the chemical features of the pharmacophore model and if the features can adopt the necessary three-dimensional arrangement to fit the model. The modeling program will indicate those features in the pharmacophore model having a fit with the particular compound or chemical feature of the compound being tested. The term "fit" when referring to a compound and a pharmacophore or binding site includes both compounds that occupy only the spatial area of the pharmacophore or binding site and compounds of which the chemical features or a portion of the molecule occupy the spatial area of the pharmacophore or binding site.

Fitting of a compound to the ligand binding site volume can be done in a number of different ways using computational methods well known by those skilled in the art. Visual inspection and manual docking of compounds into the induced-fit active site volume can be done using molecular modeling software such as QUANTA (Molecular Simulations, Burlington, MA, 1992), SYBYL (Tripos Associates, Inc., St. Louis, MO, 1992), AMBER (Weiner et al., J. Am. Chem. Soc., 106: 765-784, 1984), CHARMM (Brooks et al., J. Comp. Chem., 4: 187-217, 1983) or other modeling

programs known to those of skill in the art. This modeling step may be followed by energy minimization using standard force fields, such as CHARMM and AMBER, or others. More specialized modeling programs include MCSS (Miranker & Karplus, Function and Genetics, 11: 29-34, 1991), GRID (Goodford et al., J. Med. Chem., 28: 849-857, 1985), AUTODOCK (Goodsell & Olsen, Proteins: Structure, Function and Genetics, 8: 195-202, 1990), and DOCK (Kuntz et al., J. Mol. Biol., 161: 269-288, 1982). In addition, inhibitor compounds may be constructed *de novo* in the empty active site or in the active site including some portions of a known inhibitor using computer programs such as LEGEND (Nishibata & Itai, Tetrahedron, 47: 8985, 1991), LeapFrog (Tripos Associates, St. Louis, MO), LUDI (Bohm, J. Comp. Aid. Molec. Design, 6: 61-78, 1992), AutoLudi (Accelrys Inc., San Diego, CA) or others.

5

10

15

20

25

30

Another aspect of the invention relates to a complementary protein having a structure substantially complementary to the three-dimensional structure according to Tables 1-4; or to a medicinally effective part thereof, particularly a ligand binding region. A complementary protein is one whose three-dimensional structure is substantially complementary to the Tables 1-4 structure or a part thereof, such that the complementary structure may bind thereto and may form a complex. The lifetime of the complex may be long in the case of an inhibiting complementary protein. Of course, binding will also require an appropriate choice of amino acid sequence. Such a complementary protein may act as an inhibitor of KSP. Such inhibitors may be used *in vivo* or *in vitro* to modify the activity of KSP.

In the pharmaceutical industry, new or known compounds are routinely screened for new uses employing a variety of known *in vitro* or *in vivo* screens. Often such screens involve complex natural substances and are correspondingly expensive to carry out, and the result may be difficult to interpret. The knowledge of the three-dimensional protein structure according to the invention allows a preliminary screening to be carried out on the basis of the three-dimensional structure of a region thereof, and the structural similarity of a molecule which is being screened. This is usually carried out in conjunction with a knowledge of the amino sequence of the region. Such screening can conveniently be carried out using computer modeling techniques, which match the three-dimensional structure of the protein or part thereof (or complementary protein or part thereof) with the

structure of the molecule being screened, thereby allowing one to predict potential inhibitor activity.

The binding of a ligand to the novel binding site of the instant invention and the formation of the novel binding pocket as a result can also be indirectly assessed by spectroscopically determining the shift in the fluorescence of the amino acid 127 tryptophan residue. Thus it has been discovered that the fluorescent emission of Trp127 is modulated when KSP is treated with one of the inhibitors described above in the presence of a nucleotide or nucleotides.

A further embodiment of the instant invention is an *in vitro* assay for the determination of binding of a test compound to the novel KSP binding site described herein. The assay comprises the steps of:

- contacting KSP with the test compound and a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for Trp127 in KSP;
- contacting KSP with a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for Trp127 in KSP; and
- 3. comparing the fluorescence of the mixture of KSP, the test compound and the nucleotide with the fluorescence of the mixture of KSP with the nucleotide alone.

In another embodiment of the *in vitro* fluorescence assay the nucleotide is selected from ADP and AMPPNP (a non-hydrolysable analog of ATP, adenosine 5'- $(\beta,\gamma$ -imido)triphosphate tetralithium salt hydrate).

In an embodiment of the *in vitro* fluorescence assay the mixtures additionally contain a source of magnesium ion. Preferably the source of magnesium ion is MgCl₂.

In another embodiment of the *in vitro* fluorescence assay the measurement of the fluorescence of the KSP, test compound and nucleotide mixture is performed at several different concentrations of the test compound.

Because the KSP kinesin's three-dimensional structure is uniquely suited to the formation of the novel binding pocket of the instant invention, the methods of identification of compounds that bind to the novel binding pocket described herein, such as the fluorescence assay described

15

10

5

20

25

30

35

above, may be used to identify selective inhibitors of KSP which may not inhibit other mitotic kinesins. Such identification of a selective KSP inhibitor may offer particular advantages over an inhibitor which is competitive with the binding of the nucleotide substrate of KSP or which binds to the site of microtubule binding.

A still further aspect of the invention relates to antibodies (including monoclonal antibodies) directed to the KSP protein or complementary protein, for the detection thereof or for the modulation of its medicinal activity, it being understood that the antibody is specific for the KSP-ligand, e.g., inhibitor bound conformation.

Compounds of the structures selected or designed by any of the foregoing means may be tested for their ability to bind to a KSP protein, inhibit the binding of a KSP protein to a natural or non-natural ligand therefor, and/or inhibit a biological function mediated by a KSP protein or a BimC family member.

Finally, the present invention provides agents or inhibitors designed or selected using the methods disclosed herein. Such compounds may be utilized as described in the following sections.

Utilities

5

10

15

20

25

30

The compounds designed or selected using the methods of the invention find use in a variety of applications. As will be appreciated by those in the art, mitosis may be altered in a variety of ways; that is, one can affect mitosis either by increasing or decreasing the activity of a component in the mitotic pathway. Stated differently, mitosis may be affected (e.g., disrupted) by disturbing equilibrium, either by inhibiting or activating certain components. Similar approaches may be used to alter meiosis.

In a preferred embodiment, the compounds designed or selected using the methods of the invention are used to modulate mitotic spindle formation, thus causing prolonged cell cycle arrest in mitosis. By "modulate" herein is meant altering mitotic spindle formation, including increasing and decreasing spindle formation. By "mitotic spindle formation" herein is meant organization of microtubules into bipolar structures by mitotic kinesins. By "mitotic spindle dysfunction" herein is meant mitotic arrest and monopolar spindle formation.

The compounds designed or selected using the methods of the invention are useful to bind to and/or modulate the activity of a mitotic kinesin. In a

preferred embodiment, the mitotic kinesin is a member of the bimC subfamily of mitotic kinesins (as described in U.S. Patent No. 6,284,480, column 5). In a further preferred embodiment, the mitotic kinesin is human KSP, although the activity of mitotic kinesins from other organisms may also be modulated by the compounds of the present invention. In this context, modulate means either increasing or decreasing spindle pole separation, causing malformation, i.e., splaying, of mitotic spindle poles, or otherwise causing morphological perturbation of the mitotic spindle. Also included within the definition of KSP for these purposes are variants and/or fragments of KSP. See PCT Publ. WO 01/31335: "Methods of Screening for Modulators of Cell Proliferation and Methods of Diagnosing Cell Proliferation States", filed Oct. 27, 1999, hereby incorporated by reference in its entirety. In addition, other mitotic kinesins may be inhibited by the compounds of the present invention.

10

15

20

25

30

35

The compounds designed or selected using the methods of the invention are used to treat cellular proliferation diseases. Disease states which can be treated by the methods and compositions provided herein include, but are not limited to, cancer (further discussed below), autoimmune disease, arthritis, graft rejection, inflammatory bowel disease, proliferation induced after medical procedures, including, but not limited to, surgery, angioplasty, and the like. It is appreciated that in some cases the cells may not be in a hyper- or hypoproliferation state (abnormal state) and still require treatment. For example, during wound healing, the cells may be proliferating "normally", but proliferation enhancement may be desired. Similarly, as discussed above, in the agriculture arena, cells may be in a "normal" state, but proliferation modulation may be desired to enhance a crop by directly enhancing growth of a crop, or by inhibiting the growth of a plant or organism which adversely affects the crop. Thus, in one embodiment, the invention herein includes application to cells or individuals afflicted or impending affliction with any one of these disorders or states.

The compounds, compositions and methods provided herein are particularly deemed useful for the treatment of cancer including solid tumors such as skin, breast, brain, cervical carcinomas, testicular carcinomas, etc. More particularly, cancers that may be treated by the compounds, compositions and methods of the invention include, but are not limited to: <u>Cardiac</u>: sarcoma (angiosarcoma, fibrosarcoma, rhabdomyosarcoma, liposarcoma), myxoma, rhabdomyoma, fibroma, lipoma and teratoma; Lung: bronchogenic carcinoma (squamous cell, undifferentiated small cell, undifferentiated large cell, adenocarcinoma), alveolar (bronchiolar)

5

10

15

20

25

30

35

carcinoma, bronchial adenoma, sarcoma, lymphoma, chondromatous hamartoma, mesothelioma; Gastrointestinal: esophagus (squamous cell carcinoma, adenocarcinoma, leiomyosarcoma, lymphoma), stomach (carcinoma, lymphoma, leiomyosarcoma), pancreas (ductal adenocarcinoma, insulinoma, glucagonoma, gastrinoma, carcinoid tumors, vipoma), small bowel (adenocarcinoma, lymphoma, carcinoid tumors, Karposi's sarcoma, leiomyoma, hemangioma, lipoma, neurofibroma, fibroma), large bowel (adenocarcinoma, tubular adenoma, villous adenoma, hamartoma, leiomyoma); Genitourinary tract: kidney (adenocarcinoma, Wilm's tumor [nephroblastoma], lymphoma, leukemia), bladder and urethra (squamous cell carcinoma, transitional cell carcinoma, adenocarcinoma), prostate (adenocarcinoma, sarcoma), testis (seminoma, teratoma, embryonal carcinoma, teratocarcinoma, choriocarcinoma, sarcoma, interstitial cell carcinoma, fibroma, fibroadenoma, adenomatoid tumors, lipoma); Liver: hepatoma (hepatocellular carcinoma), cholangiocarcinoma, hepatoblastoma, angiosarcoma, hepatocellular adenoma, hemangioma; Bone: osteogenic sarcoma (osteosarcoma), fibrosarcoma, malignant fibrous histiocytoma, chondrosarcoma, Ewing's sarcoma, malignant lymphoma (reticulum cell sarcoma), multiple mycloma, malignant giant cell tumor chordoma, osteochronfroma (osteocartilaginous exostoses), benign chondroma, chondroblastoma, chondromyxofibroma, osteoid osteoma and giant cell tumors; Nervous system: skull (osteoma, hemangioma, granuloma, xanthoma, osteitis deformans), meninges (meningioma, meningiosarcoma, gliomatosis), brain (astrocytoma, medulloblastoma, glioma, ependymoma, germinoma [pinealoma], glioblastoma multiform, oligodendroglioma, schwannoma, retinoblastoma, congenital tumors), spinal cord neurofibroma, meningioma, glioma, sarcoma); Gynecological: uterus (endometrial carcinoma), cervix (cervical carcinoma, pre-tumor cervical dysplasia), ovaries (ovarian carcinoma [serous cystadenocarcinoma, mucinous cystadenocarcinoma, unclassified carcinoma], granulosa-thecal cell tumors, Sertoli-Leydig cell tumors, dysgerminoma, malignant teratoma), vulva (squamous cell carcinoma, intraepithelial carcinoma, adenocarcinoma, fibrosarcoma, melanoma), vagina (clear cell carcinoma, squamous cell carcinoma, botryoid sarcoma (embryonal rhabdomyosarcoma), fallopian tubes (carcinoma); Hematologic: blood (myeloid leukemia [acute and chronic], acute lymphoblastic leukemia, chronic lymphocytic leukemia, myeloproliferative diseases, multiple myeloma, myelodysplastic syndrome), Hodgkin's disease, non-Hodgkin's lymphoma [malignant lymphoma]; Skin: malignant melanoma, basal cell carcinoma, squamous cell carcinoma, Karposi's sarcoma, moles

dysplastic nevi, lipoma, angioma, dermatofibroma, keloids, psoriasis; and Adrenal glands: neuroblastoma. Thus, the term "cancerous cell" as provided herein, includes a cell afflicted by any one of the above-identified conditions.

The compounds designed or selected using the methods of the instant invention may also be useful as antifungal agents, by modulating the activity of the fungal members of the bimC kinesin subgroup, as is described in U.S. Patent No. 6,284,480.

5

10

15

20

25

30

35

The compounds designed or selected using the methods of this invention may be administered to mammals, preferably humans, either alone or, preferably, in combination with pharmaceutically acceptable carriers, excipients or diluents, in a pharmaceutical composition, according to standard pharmaceutical practice. The compounds can be administered orally or parenterally, including the intravenous, intramuscular, intraperitoneal, subcutaneous, rectal and topical routes of administration.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specific amounts, as well as any product which results, directly or indirectly, from combination of the specific ingredients in the specified amounts.

The pharmaceutical compositions containing the active ingredient may be in a form suitable for oral use, for example, as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules, emulsions, hard or soft capsules, or syrups or elixirs. Compositions intended for oral use may be prepared according to any method known to the art for the manufacture of pharmaceutical compositions and such compositions may contain one or more agents selected from the group consisting of sweetening agents, flavoring agents, coloring agents and preserving agents in order to provide pharmaceutically elegant and palatable preparations. Tablets contain the active ingredient in admixture with non-toxic pharmaceutically acceptable excipients which are suitable for the manufacture of tablets. These excipients may be for example, inert diluents, such as calcium carbonate, sodium carbonate, lactose, calcium phosphate or sodium phosphate; granulating and disintegrating agents, for example, microcrystalline cellulose, sodium crosscarmellose, corn starch, or alginic acid; binding agents, for example starch, gelatin, polyvinyl-pyrrolidone or acacia, and lubricating agents, for example, magnesium stearate, stearic acid or talc. The tablets may be uncoated or they may be coated by known techniques to mask the unpleasant taste of the drug or delay disintegration and absorption in the gastrointestinal tract and

thereby provide a sustained action over a longer period. For example, a water soluble taste masking material such as hydroxypropyl-methylcellulose or hydroxypropylcellulose, or a time delay material such as ethyl cellulose, cellulose acetate buryrate may be employed.

Formulations for oral use may also be presented as hard gelatin capsules wherein the active ingredient is mixed with an inert solid diluent, for example, calcium carbonate, calcium phosphate or kaolin, or as soft gelatin capsules wherein the active ingredient is mixed with water soluble carrier such as polyethyleneglycol or an oil medium, for example peanut oil, liquid paraffin, or olive oil.

5

10

15

20

25

30

Aqueous suspensions contain the active material in admixture with excipients suitable for the manufacture of aqueous suspensions. Such excipients are suspending agents, for example sodium carboxymethylcellulose, methylcellulose, hydroxypropylmethyl-cellulose, sodium alginate, polyvinyl-pyrrolidone, gum tragacanth and gum acacia; dispersing or wetting agents may be a naturally-occurring. phosphatide, for example lecithin, or condensation products of an alkylene oxide with fatty acids, for example polyoxyethylene stearate, or condensation products of ethylene oxide with long chain aliphatic alcohols, for example heptadecaethyleneoxycetanol, or condensation products of ethylene oxide with partial esters derived from fatty acids and a hexitol such as polyoxyethylene sorbitol monooleate, or condensation products of ethylene oxide with partial esters derived from fatty acids and hexitol anhydrides, for example polyethylene sorbitan monooleate. The aqueous suspensions may also contain one or more preservatives, for example ethyl, or n-propyl p-hydroxybenzoate, one or more coloring agents, one or more flavoring agents, and one or more sweetening agents, such as sucrose, saccharin or aspartame.

Oily suspensions may be formulated by suspending the active ingredient in a vegetable oil, for example arachis oil, olive oil, sesame oil or coconut oil, or in mineral oil such as liquid paraffin. The oily suspensions may contain a thickening agent, for example beeswax, hard paraffin or cetyl alcohol. Sweetening agents such as those set forth above, and flavoring agents may be added to provide a palatable oral preparation. These compositions may be preserved by the addition of an anti-oxidant such as butylated hydroxyanisol or alpha-tocopherol.

Dispersible powders and granules suitable for preparation of an aqueous suspension by the addition of water provide the active ingredient in

admixture with a dispersing or wetting agent, suspending agent and one or more preservatives. Suitable dispersing or wetting agents and suspending agents are exemplified by those already mentioned above. Additional excipients, for example sweetening, flavoring and coloring agents, may also be present. These compositions may be preserved by the addition of an anti-oxidant such as ascorbic acid.

5

10

15

20

25

30

35

The pharmaceutical compositions of the invention may also be in the form of an oil-in-water emulsions. The oily phase may be a vegetable oil, for example olive oil or arachis oil, or a mineral oil, for example liquid paraffin or mixtures of these. Suitable emulsifying agents may be naturally occurring phosphatides, for example soy bean lecithin, and esters or partial esters derived from fatty acids and hexitol anhydrides, for example sorbitan monooleate, and condensation products of the said partial esters with ethylene oxide, for example polyoxyethylene sorbitan monooleate. The emulsions may also contain sweetening, flavoring agents, preservatives and antioxidants.

Syrups and elixirs may be formulated with sweetening agents, for example glycerol, propylene glycol, sorbitol or sucrose. Such formulations may also contain a demulcent, a preservative, flavoring and coloring agents and antioxidant.

The pharmaceutical compositions may be in the form of a sterile injectable aqueous solutions. Among the acceptable vehicles and solvents that may be employed are water, Ringer's solution and isotonic sodium chloride solution.

The sterile injectable preparation may also be a sterile injectable oil-inwater microemulsion where the active ingredient is dissolved in the oily phase. For example, the active ingredient may be first dissolved in a mixture of soybean oil and lecithin. The oil solution then introduced into a water and glycerol mixture and processed to form a microemulation.

The injectable solutions or microemulsions may be introduced into a patient's blood stream by local bolus injection. Alternatively, it may be advantageous to administer the solution or microemulsion in such a way as to maintain a constant circulating concentration of the instant compound. In order to maintain such a constant concentration, a continuous intravenous delivery device may be utilized. An example of such a device is the Deltec CADD-PLUSTM model 5400 intravenous pump.

The pharmaceutical compositions may be in the form of a sterile injectable aqueous or oleagenous suspension for intramuscular and subcutaneous administration. This suspension may be formulated according to the known art using

those suitable dispersing or wetting agents and suspending agents which have been mentioned above. The sterile injectable preparation may also be a sterile injectable solution or suspension in a non-toxic parenterally acceptable diluent or solvent, for example as a solution in 1,3-butane diol. In addition, sterile, fixed oils are conventionally employed as a solvent or suspending medium. For this purpose any bland fixed oil may be employed including synthetic mono- or diglycerides. In addition, fatty acids such as oleic acid find use in the preparation of injectables.

5

10

15

20

25

30

35

Compounds designed or selected using the methods disclosed herein may also be administered in the form of suppositories for rectal administration of the drug. These compositions can be prepared by mixing the drug with a suitable non-irritating excipient which is solid at ordinary temperatures but liquid at the rectal temperature and will therefore melt in the rectum to release the drug. Such materials include cocoa butter, glycerinated gelatin, hydrogenated vegetable oils, mixtures of polyethylene glycols of various molecular weights and fatty acid esters of polyethylene glycol.

For topical use, creams, ointments, jellies, solutions or suspensions, etc., containing the compound are employed. (For purposes of this application, topical application shall include mouth washes and gargles.)

The compounds designed or selected using the methods of the present invention can be administered in intranasal form via topical use of suitable intranasal vehicles and delivery devices, or via transdermal routes, using those forms of transdermal skin patches well known to those of ordinary skill in the art. To be administered in the form of a transdermal delivery system, the dosage administration will, of course, be continuous rather than intermittent throughout the dosage regimen. Compounds of the present invention may also be delivered as a suppository

compounds of the present invention may also be delivered as a suppository employing bases such as cocoa butter, glycerinated gelatin, hydrogenated vegetable oils, mixtures of polyethylene glycols of various molecular weights and fatty acid esters of polyethylene glycol.

When a compound according to this invention is administered into a human subject, the daily dosage will normally be determined by the prescribing physician with the dosage generally varying according to the age, weight, sex and response of the individual patient, as well as the severity of the patient's symptoms.

In one exemplary application, a suitable amount of compound is administered to a mammal undergoing treatment for cancer. Administration occurs in an amount between about 0.1 mg/kg of body weight to about 60 mg/kg of body

5

10

15

20

25

30

weight per day, preferably of between 0.5 mg/kg of body weight to about 40 mg/kg of body weight per day.

The compounds designed or selected using the methods disclosed herein (hereafter referred to as the "instant compounds") are also useful in combination with known therapeutic agents and anti-cancer agents. For example, instant compounds are useful in combination with known anti-cancer agents. Combinations of the presently disclosed compounds with other anti-cancer or chemotherapeutic agents are within the scope of the invention. Examples of such agents can be found in Cancer Principles and Practice of Oncology by V.T. Devita and S. Hellman (editors), 6th edition (February 15, 2001), Lippincott Williams & Wilkins Publishers. A person of ordinary skill in the art would be able to discern which combinations of agents would be useful based on the particular characteristics of the drugs and the cancer involved. Such anti-cancer agents include, but are not limited to, the following: estrogen receptor modulators, androgen receptor modulators, retinoid receptor modulators, cytotoxic/cytostatic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors and other angiogenesis inhibitors, inhibitors of cell proliferation and survival signaling, and agents that interfere with cell cycle checkpoints. The instant compounds are particularly useful when co-administered with radiation therapy.

In an embodiment, the instant compounds are also useful in combination with known anti-cancer agents including the following: estrogen receptor modulators, androgen receptor modulators, retinoid receptor modulators, cytotoxic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors, HIV protease inhibitors, reverse transcriptase inhibitors, and other angiogenesis inhibitors.

"Estrogen receptor modulators" refers to compounds that interfere with or inhibit the binding of estrogen to the receptor, regardless of mechanism. Examples of estrogen receptor modulators include, but are not limited to, tamoxifen, raloxifene, idoxifene, LY353381, LY117081, toremifene, fulvestrant, 4-[7-(2,2-dimethyl-1-oxopropoxy-4-methyl-2-[4-[2-(1-piperidinyl)ethoxy]phenyl]-2H-1-benzopyran-3-yl]-phenyl-2,2-dimethylpropanoate, 4,4'-dihydroxybenzophenone-2,4-dinitrophenyl-hydrazone, and SH646.

"Androgen receptor modulators" refers to compounds which interfere or inhibit the binding of androgens to the receptor, regardless of mechanism.

Examples of androgen receptor modulators include finasteride and other 5α -reductase inhibitors, nilutamide, flutamide, bicalutamide, liarozole, and abiraterone acetate.

"Retinoid receptor modulators" refers to compounds which interfere or inhibit the binding of retinoids to the receptor, regardless of mechanism. Examples of such retinoid receptor modulators include bexarotene, tretinoin, 13-cis-retinoic acid, 9-cis-retinoic acid, α-difluoromethylornithine, ILX23-7553, trans-N-(4'-hydroxyphenyl) retinamide, and N-4-carboxyphenyl retinamide.

5

10

15

20

25

30

35

"Cytotoxic/cytostatic agents" refer to compounds which cause cell death or inhibit cell proliferation primarily by interfering directly with the cell's functioning or inhibit or interfere with cell myosis, including alkylating agents, tumor necrosis factors, intercalators, hypoxia activatable compounds, microtubule inhibitors/microtubule-stabilizing agents, inhibitors of mitotic kinesins, inhibitors of kinases involved in mitotic progression, antimetabolites; biological response modifiers; hormonal/anti-hormonal therapeutic agents, haematopoietic growth factors, monoclonal antibody targeted therapeutic agents, topoisomerase inhibitors, proteosome inhibitors and ubiquitin ligase inhibitors.

Examples of cytotoxic agents include, but are not limited to, sertenef, cachectin, ifosfamide, tasonermin, lonidamine, carboplatin, altretamine, prednimustine, dibromodulcitol, ranimustine, fotemustine, nedaplatin, oxaliplatin, temozolomide, heptaplatin, estramustine, improsulfan tosilate, trofosfamide, nimustine, dibrospidium chloride, pumitepa, lobaplatin, satraplatin, profiromycin, cisplatin, irofulven, dexifosfamide, cis-aminedichloro(2-methyl-pyridine)platinum, benzylguanine, glufosfamide, GPX100, (trans, trans, trans)-bis-mu-(hexane-1,6-diamine)-mu-[diamine-platinum(II)]bis[diamine(chloro)platinum (II)]tetrachloride, diarizidinylspermine, arsenic trioxide, 1-(11-dodecylamino-10-hydroxyundecyl)-3,7-dimethylxanthine, zorubicin, idarubicin, daunorubicin, bisantrene, mitoxantrone, pirarubicin, pinafide, valrubicin, amrubicin, antineoplaston, 3'-deamino-3'-morpholino-13-deoxo-10-hydroxycarminomycin, annamycin, galarubicin, elinafide, MEN10755, and 4-demethoxy-3-deamino-3-aziridinyl-4-methylsulphonyl-daunorubicin (see WO 00/50032).

An example of a hypoxia activatable compound is tirapazamine.

Examples of proteosome inhibitors include but are not limited to lactacystin and MLN-341 (Velcade).

Examples of microtubule inhibitors/microtubule-stabilising agents include paclitaxel, vindesine sulfate, 3',4'-didehydro-4'-deoxy-8'-

norvincaleukoblastine, docetaxol, rhizoxin, dolastatin, mivobulin isethionate, auristatin, cemadotin, RPR109881, BMS184476, vinflunine, cryptophycin, 2,3,4,5,6-pentafluoro-N-(3-fluoro-4-methoxyphenyl) benzene sulfonamide, anhydrovinblastine, N,N-dimethyl-L-valyl-L-valyl-L-valyl-L-prolyl-L-proline-t-butylamide,

TDX258, the epothilones (see for example U.S. Pat. Nos. 6,284,781 and 6,288,237) and BMS188797. In an embodiment the epothilones are not included in the microtubule inhibitors/microtubule-stabilising agents.

Some examples of topoisomerase inhibitors are topotecan, hycaptamine, irinotecan, rubitecan, 6-ethoxypropionyl-3',4'-O-exo-benzylidene-chartreusin, 9-methoxy-N,N-dimethyl-5-nitropyrazolo[3,4,5-kl]acridine-2-(6H) propanamine, 1-amino-9-ethyl-5-fluoro-2,3-dihydro-9-hydroxy-4-methyl-1H,12H-benzo[de]pyrano[3',4':b,7]-indolizino[1,2b]quinoline-10,13(9H,15H)dione, lurtotecan, 7-[2-(N-isopropylamino)ethyl]-(20S)camptothecin, BNP1350, BNPI1100, BN80915, BN80942, etoposide phosphate, teniposide, sobuzoxane, 2'-

- dimethylamino-2'-deoxy-etoposide, GL331, N-[2-(dimethylamino)ethyl]-9-hydroxy-5,6-dimethyl-6H-pyrido[4,3-b]carbazole-1-carboxamide, asulacrine, (5a, 5aB, 8aa,9b)-9-[2-[N-[2-(dimethylamino)ethyl]-N-methylamino]ethyl]-5-[4-hydro0xy-3,5-dimethoxyphenyl]-5,5a,6,8,8a,9-hexohydrofuro(3',4':6,7)naphtho(2,3-d)-1,3-dioxol-6-one, 2,3-(methylenedioxy)-5-methyl-7-hydroxy-8-methoxybenzo[c]-
- phenanthridinium, 6,9-bis[(2-aminoethyl)amino]benzo[g]isoguinoline-5,10-dione, 5-(3-aminopropylamino)-7,10-dihydroxy-2-(2-hydroxyethylaminomethyl)-6H-pyrazolo[4,5,1-de]acridin-6-one, N-[1-[2(diethylamino)ethylamino]-7-methoxy-9-oxo-9H-thioxanthen-4-ylmethyl]formamide, N-(2-(dimethylamino)ethyl)acridine-4-carboxamide, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-7H-indeno[2,1-c] quinolin-7-one, and dimesna.

Examples of inhibitors of mitotic kinesins, and in particular the human mitotic kinesin KSP, are described in PCT Publications WO 01/30768 and WO 01/98278, and pending U.S. Ser. Nos. 60/338,779 (filed December 6, 2001), 60/338,344 (filed December 6, 2001), 60/338,383 (filed December 6, 2001), 60/338,380 (filed December 6, 2001), 60/338,379 (filed December 6, 2001) and 60/344,453 (filed November 7, 2001). In an embodiment inhibitors of mitotic kinesins include, but are not limited to inhibitors of KSP, inhibitors of MKLP1, inhibitors of CENP-E, inhibitors of MCAK and inhibitors of Rab6-KIFL.

30

"Inhibitors of kinases involved in mitotic progression" include, but are not limited to, inhibitors of aurora kinase, inhibitors of Polo-like kinases (PLK) (in particular inhibitors of PLK-1), inhibitors of bub-1 and inhibitors of bub-R1.

"Antiproliferative agents" includes antisense RNA and DNA oligonucleotides such as G3139, ODN698, RVASKRAS, GEM231, and INX3001, 5 and antimetabolites such as enocitabine, carmofur, tegafur, pentostatin, doxifluridine, trimetrexate, fludarabine, capecitabine, galocitabine, cytarabine ocfosfate, fosteabine sodium hydrate, raltitrexed, paltitrexid, emitefur, tiazofurin, decitabine, nolatrexed, pemetrexed, nelzarabine, 2'-deoxy-2'-methylidenecytidine, 2'-fluoromethylene-2'-10 deoxycytidine, N-[5-(2,3-dihydro-benzofuryl)sulfonyl]-N'-(3,4-dichlorophenyl)urea, N6-[4-deoxy-4-[N2-[2(E),4(E)-tetradecadienoyl]glycylamino]-L-glycero-B-L-mannoheptopyranosyl]adenine, aplidine, ecteinascidin, troxacitabine, 4-[2-amino-4-oxo-4,6,7,8-tetrahydro-3H-pyrimidino[5,4-b][1,4]thiazin-6-yl-(S)-ethyl]-2,5-thienoyl-Lglutamic acid, aminopterin, 5-flurouracil, alanosine, 11-acetyl-8-15 (carbamoyloxymethyl)-4-formyl-6-methoxy-14-oxa-1,11-diazatetracyclo(7.4.1.0.0)tetradeca-2,4,6-trien-9-yl acetic acid ester, swainsonine, lometrexol, dexrazoxane, methioninase, 2'-cyano-2'-deoxy-N4-palmitoyl-1-B-D-arabino furanosyl cytosine, 3-

Examples of monoclonal antibody targeted therapeutic agents include those therapeutic agents which have cytotoxic agents or radioisotopes attached to a cancer cell specific or target cell specific monoclonal antibody. Examples include Bexxar.

aminopyridine-2-carboxaldehyde thiosemicarbazone and trastuzumab.

20

25

"HMG-CoA reductase inhibitors" refers to inhibitors of 3-hydroxy-3-methylglutaryl-CoA reductase. Compounds which have inhibitory activity for HMG-CoA reductase can be readily identified by using assays well-known in the art. For example, see the assays described or cited in U.S. Patent 4,231,938 at col. 6, and WO 84/02131 at pp. 30-33. The terms "HMG-CoA reductase inhibitor" and "inhibitor of HMG-CoA reductase" have the same meaning when used herein.

Examples of HMG-CoA reductase inhibitors that may be used include but are not limited to lovastatin (MEVACOR®; see U.S. Patent Nos. 4,231,938, 4,294,926 and 4,319,039), simvastatin (ZOCOR®; see U.S. Patent Nos. 4,444,784, 4,820,850 and 4,916,239), pravastatin (PRAVACHOL®; see U.S. Patent Nos. 4,346,227, 4,537,859, 4,410,629, 5,030,447 and 5,180,589), fluvastatin (LESCOL®; see U.S. Patent Nos. 5,354,772, 4,911,165, 4,929,437, 5,189,164, 5,118,853, 5,290,946 and 5,356,896), atorvastatin (LIPITOR®; see U.S. Patent Nos. 5,273,995,

4,681,893, 5,489,691 and 5,342,952) and cerivastatin (also known as rivastatin and BAYCHOL®; see US Patent No. 5,177,080). The structural formulas of these and additional HMG-CoA reductase inhibitors that may be used in the instant methods are described at page 87 of M. Yalpani, "Cholesterol Lowering Drugs", *Chemistry & Industry*, pp. 85-89 (5 February 1996) and US Patent Nos. 4,782,084 and 4,885,314. The term HMG-CoA reductase inhibitor as used herein includes all pharmaceutically acceptable lactone and open-acid forms (i.e., where the lactone ring is opened to form the free acid) as well as salt and ester forms of compounds which have HMG-CoA reductase inhibitory activity, and therefor the use of such salts, esters, open-acid and lactone forms is included within the scope of this invention. An illustration of the lactone portion and its corresponding open-acid form is shown below as structures I and II.

5

10

15

20

25

In HMG-CoA reductase inhibitors where an open-acid form can exist, salt and ester forms may be formed from the open-acid, and all such forms are included within the meaning of the term "HMG-CoA reductase inhibitor" as used herein. In an embodiment, the HMG-CoA reductase inhibitor is selected from lovastatin and simvastatin, and in a further embodiment, simvastatin. Herein, the term "pharmaceutically acceptable salts" with respect to the HMG-CoA reductase inhibitor shall mean non-toxic salts of the compounds employed in this invention which are generally prepared by reacting the free acid with a suitable organic or inorganic base, particularly those formed from cations such as sodium, potassium, aluminum, calcium, lithium, magnesium, zinc and tetramethylammonium, as well as those salts formed from amines such as ammonia, ethylenediamine, N-methylglucamine, lysine, arginine, ornithine, choline, N,N'-dibenzylethylenediamine, chloroprocaine, diethanolamine, procaine, N-benzylphenethylamine, 1-p-

chlorobenzyl-2-pyrrolidine-1'-yl-methylbenz-imidazole, diethylamine, piperazine, and tris(hydroxymethyl) aminomethane. Further examples of salt forms of HMG-CoA reductase inhibitors may include, but are not limited to, acetate, benzenesulfonate, benzoate, bicarbonate, bisulfate, bitartrate, borate, bromide, calcium edetate, camsylate, carbonate, chloride, clavulanate, citrate, dihydrochloride, edetate, edisylate, estolate, esylate, fumarate, gluceptate, gluconate, glutamate, glycollylarsanilate, hexylresorcinate, hydrabamine, hydrobromide, hydrochloride, hydroxynapthoate, iodide, isothionate, lactate, lactobionate, laurate, malate, maleate, mandelate, mesylate, methylsulfate, mucate, napsylate, nitrate, oleate, oxalate, pamaote, palmitate, panthothenate, phosphate/diphosphate, polygalacturonate, salicylate, stearate, subacetate, succinate, tannate, tartrate, teoclate, tosylate, triethiodide, and valerate.

5

10

15

Ester derivatives of the described HMG-CoA reductase inhibitor compounds may act as prodrugs which, when absorbed into the bloodstream of a warm-blooded animal, may cleave in such a manner as to release the drug form and permit the drug to afford improved therapeutic efficacy.

"Prenyl-protein transferase inhibitor" refers to a compound which inhibits any one or any combination of the prenyl-protein transferase enzymes, including farnesyl-protein transferase (FPTase), geranylgeranyl-protein transferase 20 type I (GGPTase-I), and geranylgeranyl-protein transferase type-II (GGPTase-II, also called Rab GGPTase). Examples of prenyl-protein transferase inhibiting compounds include (+)-6-[amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl)methyl]-4-(3chlorophenyl)-1-methyl-2(1H)-quinolinone, (-)-6-[amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl)methyl]-4-(3-chlorophenyl)-1-methyl-2(1H)-quinolinone, (+)-6-25 [amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl) methyl]-4-(3-chlorophenyl)-1methyl-2(1H)-quinolinone, 5(S)-n-butyl-1-(2,3-dimethylphenyl)-4-[1-(4cyanobenzyl)-5-imidazolylmethyl]-2-piperazinone, (S)-1-(3-chlorophenyl) -4-[1-(4cyanobenzyl)-5-imidazolylmethyl]-5-[2-(ethanesulfonyl) methyl)-2-piperazinone, 5(S)-n-Butyl-1-(2-methylphenyl)-4-[1-(4-cyanobenzyl)-5-imidazolylmethyl]-2-30 piperazinone, 1-(3-chlorophenyl) -4-[1-(4-cyanobenzyl)-2-methyl-5imidazolylmethyl]-2-piperazinone, 1-(2,2-diphenylethyl)-3-[N-(1-(4-cyanobenzyl)-1H-imidazol-5-ylethyl)carbamoyl]piperidine, 4-{5-[4-hydroxymethyl-4-(4chloropyridin-2-ylmethyl)-piperidine-1-ylmethyl]-2-methylimidazol-1-ylmethyl} benzonitrile, 4-{5-[4-hydroxymethyl-4-(3-chlorobenzyl)-piperidine-1-ylmethyl]-2methylimidazol-1-ylmethyl}benzonitrile, 4-{3-[4-(2-oxo-2H-pyridin-1-yl)benzyl]-3H-35

imidazol-4-ylmethyl) benzonitrile, 4-{3-[4-(5-chloro-2-oxo-2H-[1,2'] bipyridin-5'-ylmethyl]-3H-imidazol-4-ylmethyl} benzonitrile, 4-{3-[4-(2-oxo-2H-[1,2'] bipyridin-5'-ylmethyl]-3H-imidazol-4-ylmethyl} benzonitrile, 4-[3-(2-oxo-1-phenyl-1,2-dihydropyridin-4-ylmethyl)-3H-imidazol-4-ylmethyl} benzonitrile, 18,19-dihydro-19-oxo-5H,17H-6,10:12,16-dimetheno-1H-imidazo[4,3-c][1,11,4]dioxaazacyclononadecine-9-carbonitrile, (±)-19,20-dihydro-19-oxo-5H-18,21-ethano-12,14-etheno-6,10-metheno-22H-benzo[d]imidazo[4,3-k][1,6,9,12]oxatriaza-cyclooctadecine-9-carbonitrile, 19,20-dihydro-19-oxo-5H,17H-18,21-ethano-6,10:12,16-dimetheno-22H-imidazo[3,4-h][1,8,11,14]oxatriazacycloeicosine-9-carbonitrile, and (±)-19,20-dihydro-3-methyl-19-oxo-5H-18,21-ethano-12,14-etheno-6,10-metheno-22H-benzo [d]imidazo[4,3-k][1,6,9,12]oxa-triazacyclooctadecine-9-carbonitrile.

5

10

30

Other examples of prenyl-protein transferase inhibitors can be found in the following publications and patents: WO 96/30343, WO 97/18813, WO 97/21701, WO 97/23478, WO 97/38665, WO 98/28980, WO 98/29119, WO 95/32987,

- U.S. Patent No. 5,420,245, U.S. Patent No. 5,523,430, U.S. Patent No. 5,532,359,
 U.S. Patent No. 5,510,510, U.S. Patent No. 5,589,485, U.S. Patent No. 5,602,098,
 European Patent Publ. 0 618 221, European Patent Publ. 0 675 112, European Patent
 Publ. 0 604 181, European Patent Publ. 0 696 593, WO 94/19357, WO 95/08542, WO 95/11917, WO 95/12612, WO 95/12572, WO 95/10514, U.S. Patent No. 5,661,152,
- 20 WO 95/10515, WO 95/10516, WO 95/24612, WO 95/34535, WO 95/25086, WO 96/05529, WO 96/06138, WO 96/06193, WO 96/16443, WO 96/21701, WO 96/21456, WO 96/22278, WO 96/24611, WO 96/24612, WO 96/05168, WO 96/05169, WO 96/00736, U.S. Patent No. 5,571,792, WO 96/17861, WO 96/33159, WO 96/34850, WO 96/34851, WO 96/30017, WO 96/30018, WO 96/30362, WO
- 25 96/30363, WO 96/31111, WO 96/31477, WO 96/31478, WO 96/31501, WO 97/00252, WO 97/03047, WO 97/03050, WO 97/04785, WO 97/02920, WO 97/17070, WO 97/23478, WO 97/26246, WO 97/30053, WO 97/44350, WO 98/02436, and U.S. Patent No. 5,532,359.

For an example of the role of a prenyl-protein transferase inhibitor on angiogenesis see European J. of Cancer, Vol. 35, No. 9, pp.1394-1401 (1999).

"Angiogenesis inhibitors" refers to compounds that inhibit the formation of new blood vessels, regardless of mechanism. Examples of angiogenesis inhibitors include, but are not limited to, tyrosine kinase inhibitors, such as inhibitors of the tyrosine kinase receptors Flt-1 (VEGFR1) and Flk-1/KDR (VEGFR2),

35 inhibitors of epidermal-derived, fibroblast-derived, or platelet derived growth factors,

MMP (matrix metalloprotease) inhibitors, integrin blockers, interferon-α, interleukin-12, pentosan polysulfate, cyclooxygenase inhibitors, including nonsteroidal anti-inflammatories (NSAIDs) like aspirin and ibuprofen as well as selective cyclooxygenase-2 inhibitors like celecoxib and rofecoxib (PNAS, Vol. 89, p. 7384 (1992);

- JNCI, Vol. 69, p. 475 (1982); Arch. Opthalmol., Vol. 108, p.573 (1990); Anat. Rec.,
 Vol. 238, p. 68 (1994); FEBS Letters, Vol. 372, p. 83 (1995); Clin, Orthop. Vol. 313,
 p. 76 (1995); J. Mol. Endocrinol., Vol. 16, p.107 (1996); Jpn. J. Pharmacol., Vol. 75,
 p. 105 (1997); Cancer Res., Vol. 57, p. 1625 (1997); Cell, Vol. 93, p. 705 (1998); Intl.
 J. Mol. Med., Vol. 2, p. 715 (1998); J. Biol. Chem., Vol. 274, p. 9116 (1999)),
- steroidal anti-inflammatories (such as corticosteroids, mineralocorticoids, dexamethasone, prednisone, prednisolone, methylpred, betamethasone), carboxyamidotriazole, combretastatin A-4, squalamine, 6-O-chloroacetyl-carbonyl)-fumagillol, thalidomide, angiostatin, troponin-1, angiotensin II antagonists (see Fernandez et al., J. Lab. Clin. Med. 105:141-145 (1985)), and antibodies to VEGF
 (see, Nature Biotechnology, Vol. 17, pp.963-968 (October 1999); Kim et al., Nature, 362, 841-844 (1993); WO 00/44777; and WO 00/61186).

Other therapeutic agents that modulate or inhibit angiogenesis and may also be used in combination with the compounds of the instant invention include agents that modulate or inhibit the coagulation and fibrinolysis systems (see review in Clin. Chem. La. Med. 38:679-692 (2000)). Examples of such agents that modulate or inhibit the coagulation and fibrinolysis pathways include, but are not limited to, heparin (see Thromb. Haemost. 80:10-23 (1998)), low molecular weight heparins, GPIIb/IIIa antagonists (such as tirofiban), warfarin, thrombin inhibitors and carboxypeptidase U inhibitors (also known as inhibitors of active thrombin activatable fibrinolysis inhibitor [TAFIa]) (see Thrombosis Res. 101:329-354 (2001)). TAFIa inhibitors have been described in U.S. Serial Nos. 60/310,927 (filed August 8, 2001) and 60/349,925 (filed January 18, 2002).

"Agents that interfere with cell cycle checkpoints" refer to compounds that inhibit protein kinases that transduce cell cycle checkpoint signals, thereby sensitizing the cancer cell to DNA damaging agents. Such agents include inhibitors of ATR, ATM, the Chk1 and Chk2 kinases and cdk and cdc kinase inhibitors and are specifically exemplified by 7-hydroxystaurosporin, flavopiridol, CYC202 (Cyclacel) and BMS-387032.

30

"Inhibitors of cell proliferation and survival signalling pathway" refer to compounds that inhibit signal transduction cascades downstream of cell surface receptors. Such agents include inhibitors of serine/threonine kinases (including but not limited to inhibitors of Akt such as described in WO 02/083064, WO 02/083139, WO 02/083140 and WO 02/083138), inhibitors of Raf kinase (for example BAY-43-9006), inhibitors of MEK (for example CI-1040 and PD-098059), inhibitors of mTOR (for example Wyeth CCI-779), and inhibitors of PI3K (for example LY294002).

The combinations with NSAID's are directed to the use of NSAID's which are potent COX-2 inhibiting agents. For purposes of this specification an NSAID is potent if it possess an IC₅₀ for the inhibition of COX-2 of $1\mu M$ or less as measured by cell or microsomal assays.

The invention also encompasses combinations with NSAID's which are selective COX-2 inhibitors. For purposes of this specification NSAID's which are 15 selective inhibitors of COX-2 are defined as those which possess a specificity for inhibiting COX-2 over COX-1 of at least 100 fold as measured by the ratio of IC50 for COX-2 over IC50 for COX-1 evaluated by cell or microsomal assays. Such compounds include, but are not limited to those disclosed in U.S. Patent 5,474,995, issued December 12, 1995, U.S. Patent 5,861,419, issued January 19, 1999, U.S. 20 Patent 6,001,843, issued December 14, 1999, U.S. Patent 6,020,343, issued February 1, 2000, U.S. Patent 5,409,944, issued April 25, 1995, U.S. Patent 5,436,265, issued July 25, 1995, U.S. Patent 5,536,752, issued July 16, 1996, U.S. Patent 5,550,142, issued August 27, 1996, U.S. Patent 5,604,260, issued February 18, 1997, U.S. 5,698,584, issued December 16, 1997, U.S. Patent 5,710,140, issued January 20,1998, 25 WO 94/15932, published July 21, 1994, U.S. Patent 5,344,991, issued June 6, 1994, U.S. Patent 5,134,142, issued July 28, 1992, U.S. Patent 5,380,738, issued January 10, 1995, U.S. Patent 5,393,790, issued February 20, 1995, U.S. Patent 5,466,823, issued November 14, 1995, U.S. Patent 5,633,272, issued May 27, 1997, and U.S. Patent 5,932,598, issued August 3, 1999, all of which are hereby incorporated by 30 reference.

Inhibitors of COX-2 that are particularly useful in the instant method of treatment are:

3-phenyl-4-(4-(methylsulfonyl)phenyl)-2-(5H)-furanone; and

10

5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine;

5

10

15

or a pharmaceutically acceptable salt thereof.

General and specific synthetic procedures for the preparation of the COX-2 inhibitor compounds described above are found in U.S. Patent No. 5,474,995, issued December 12, 1995, U.S. Patent No. 5,861,419, issued January 19, 1999, and U.S. Patent No. 6,001,843, issued December 14, 1999, all of which are herein incorporated by reference.

Compounds that have been described as specific inhibitors of COX-2 and are therefore useful in the present invention include, but are not limited to, the following:

$$\begin{array}{c|c}
O & O \\
H_2N & & N \\
H_3C & O \\
H_2N - S & O \\
\hline
H_3C & O \\
\hline$$

or a pharmaceutically acceptable salt thereof.

5

10

Compounds which are described as specific inhibitors of COX-2 and are therefore useful in the present invention, and methods of synthesis thereof, can be found in the following patents, pending applications and publications, which are herein incorporated by reference: WO 94/15932, published July 21, 1994, U.S. Patent No. 5,344,991, issued June 6, 1994, U.S. Patent No. 5,134,142, issued July 28, 1992, U.S. Patent No. 5,380,738, issued January 10, 1995, U.S. Patent No. 5,393,790, issued February 20, 1995, U.S. Patent No. 5,466,823, issued November 14, 1995, U.S. Patent No. 5,633,272, issued May 27, 1997, and U.S. Patent No. 5,932,598, issued August 3, 1999.

Compounds which are specific inhibitors of COX-2 and are therefore useful in the present invention, and methods of synthesis thereof, can be found in the following patents, pending applications and publications, which are herein incorporated by reference: U.S. Patent No. 5,474,995, issued December 12, 1995, U.S. Patent No. 5,861,419, issued January 19, 1999, U.S. Patent No. 6,001,843, issued December 14, 1999, U.S. Patent No. 6,020,343, issued February 1, 2000, U.S. Patent No. 5,409,944, issued April 25, 1995, U.S. Patent No. 5,436,265, issued July 25, 1995, U.S. Patent No. 5,536,752, issued July 16, 1996, U.S. Patent No. 5,550,142, issued August 27, 1996, U.S. Patent No. 5,604,260, issued February 18, 1997, U.S. Patent No. 5,698,584, issued December 16, 1997, and U.S. Patent No. 5,710,140, issued January 20,1998.

5

10

20

25

30

35

Other examples of angiogenesis inhibitors include, but are not limited to, endostatin, ukrain, ranpirnase, IM862, 5-methoxy-4-[2-methyl-3-(3-methyl-2-butenyl)oxiranyl]-1-oxaspiro[2,5]oct-6-yl(chloroacetyl)carbamate, acetyldinanaline, 5-amino-1-[[3,5-dichloro-4-(4-chlorobenzoyl)phenyl]methyl]-1H-1,2,3-triazole-4-carboxamide,CM101, squalamine, combretastatin, RPI4610, NX31838, sulfated mannopentaose phosphate, 7,7-(carbonyl-bis[imino-N-methyl-4,2-pyrrolocarbonylimino[N-methyl-4,2-pyrrole]-carbonylimino]-bis-(1,3-naphthalene disulfonate), and 3-[(2,4-dimethylpyrrol-5-yl)methylene]-2-indolinone (SU5416).

As used above, "integrin blockers" refers to compounds which selectively antagonize, inhibit or counteract binding of a physiological ligand to the $\alpha_V\beta_3$ integrin, to compounds which selectively antagonize, inhibit or counteract binding of a physiological ligand to the $\alpha_V\beta_5$ integrin, to compounds which antagonize, inhibit or counteract binding of a physiological ligand to both the $\alpha_V\beta_3$ integrin and the $\alpha_V\beta_5$ integrin, and to compounds which antagonize, inhibit or counteract the activity of the particular integrin(s) expressed on capillary endothelial cells. The term also refers to antagonists of the $\alpha_V\beta_6$, $\alpha_V\beta_8$, $\alpha_1\beta_1$, $\alpha_2\beta_1$, $\alpha_5\beta_1$, $\alpha_6\beta_1$ and $\alpha_6\beta_4$ integrins. The term also refers to antagonists of any combination of $\alpha_V\beta_3$, $\alpha_V\beta_5$, $\alpha_V\beta_6$, $\alpha_V\beta_8$, $\alpha_1\beta_1$, $\alpha_2\beta_1$, $\alpha_5\beta_1$, $\alpha_6\beta_1$ and $\alpha_6\beta_4$ integrins.

Some specific examples of tyrosine kinase inhibitors include N-(trifluoromethylphenyl)-5-methylisoxazol-4-carboxamide, 3-[(2,4-dimethylpyrrol-5-yl)methylidenyl)indolin-2-one, 17-(allylamino)-17-demethoxygeldanamycin, 4-(3-chloro-4-fluorophenylamino)-7-methoxy-6-[3-(4-morpholinyl)propoxyl]quinazoline, N-(3-ethynylphenyl)-6,7-bis(2-methoxyethoxy)-4-quinazolinamine, BIBX1382, 2,3,9,10,11,12-hexahydro-10-(hydroxymethyl)-10-hydroxy-9-methyl-9,12-epoxy-1H-

diindolo[1,2,3-fg:3',2',1'-kl]pyrrolo[3,4-i][1,6]benzodiazocin-1-one, SH268, genistein, STI571, CEP2563, 4-(3-chlorophenylamino)-5,6-dimethyl-7H-pyrrolo[2,3-d]pyrimidinemethane sulfonate, 4-(3-bromo-4-hydroxyphenyl)amino-6,7-dimethoxyquinazoline, 4-(4'-hydroxyphenyl)amino-6,7-dimethoxyquinazoline, SU6668, STI571A, N-4-chlorophenyl-4-(4-pyridylmethyl)-1-phthalazinamine, and EMD121974.

5

30

Combinations with compounds other than anti-cancer compounds are also encompassed in the instant methods. For example, combinations of the instantly claimed compounds with PPAR-γ (i.e., PPAR-gamma) agonists and PPAR-δ (i.e., 10 PPAR-delta) agonists are useful in the treatment of certain malingnancies. PPAR-y and PPAR- δ are the nuclear peroxisome proliferator-activated receptors γ and δ . The expression of PPAR-y on endothelial cells and its involvement in angiogenesis has been reported in the literature (see J. Cardiovasc. Pharmacol. 1998; 31:909-913; J. Biol. Chem. 1999;274:9116-9121; Invest. Ophthalmol Vis. Sci. 2000; 41:2309-2317). 15 More recently, PPAR-y agonists have been shown to inhibit the angiogenic response to VEGF in vitro; both troglitazone and rosiglitazone maleate inhibit the development of retinal neovascularization in mice. (Arch. Ophthamol. 2001; 119:709-717). Examples of PPAR-γ agonists and PPAR-γ/α agonists include, but are not limited to, thiazolidinediones (such as DRF2725, CS-011, troglitazone, rosiglitazone, and 20 pioglitazone), fenofibrate, gemfibrozil, clofibrate, GW2570, SB219994, AR-H039242, JTT-501, MCC-555, GW2331, GW409544, NN2344, KRP297, NP0110, DRF4158, NN622, GI262570, PNU182716, DRF552926, 2-[(5,7-dipropyl-3trifluoromethyl-1,2-benzisoxazol-6-yl)oxyl-2-methylpropionic acid (disclosed in USSN 09/782,856), and 2(R)-7-(3-(2-chloro-4-(4-fluorophenoxy) phenoxy)propoxy)-25 2-ethylchromane-2-carboxylic acid (disclosed in USSN 60/235,708 and 60/244,697).

Another embodiment of the instant invention is the use of the presently disclosed compounds in combination with gene therapy for the treatment of cancer. For an overview of genetic strategies to treating cancer see Hall et al (Am J Hum Genet 61:785-789, 1997) and Kufe et al (Cancer Medicine, 5th Ed, pp 876-889, BC Decker, Hamilton 2000). Gene therapy can be used to deliver any tumor suppressing gene. Examples of such genes include, but are not limited to, p53, which can be delivered via recombinant virus-mediated gene transfer (see U.S. Patent No. 6,069,134, for example), a uPA/uPAR antagonist ("Adenovirus-Mediated Delivery of a uPA/uPAR Antagonist Suppresses Angiogenesis-Dependent Tumor Growth and

Dissemination in Mice," Gene Therapy, August 1998;5(8):1105-13), and interferon gamma (J Immunol 2000;164:217-222).

The compounds designed or selected using the methods of the instant invention may also be administered in combination with an inhibitor of inherent multidrug resistance (MDR), in particular MDR associated with high levels of expression of transporter proteins. Such MDR inhibitors include inhibitors of pglycoprotein (P-gp), such as LY335979, XR9576, OC144-093, R101922, VX853 and PSC833 (valspodar).

5

15

20

25

30

A compound designed or selected using the methods of the present invention may be employed in conjunction with anti-emetic agents to treat nausea or 10 emesis, including acute, delayed, late-phase, and anticipatory emesis, which may result from the use of a compound of the present invention, alone or with radiation therapy. For the prevention or treatment of emesis, a compound of the present invention may be used in conjunction with other anti-emetic agents, especially neurokinin-1 receptor antagonists, 5HT3 receptor antagonists, such as ondansetron, granisetron, tropisetron, and zatisetron, GABAB receptor agonists, such as baclofen, a corticosteroid such as Decadron (dexamethasone), Kenalog, Aristocort, Nasalide, Preferid, Benecorten or others such as disclosed in U.S.Patent Nos. 2,789,118, 2,990,401, 3,048,581, 3,126,375, 3,929,768, 3,996,359, 3,928,326 and 3,749,712, an antidopaminergic, such as the phenothiazines (for example prochlorperazine, fluphenazine, thioridazine and mesoridazine), metoclopramide or dronabinol. For the treatment or prevention of emesis that may result upon administration of the instant compounds, conjunctive therapy with an anti-emesis agent selected from a neurokinin-1 receptor antagonist, a 5HT3 receptor antagonist and a corticosteroid is preferred.

Neurokinin-1 receptor antagonists of use in conjunction with the compounds of the present invention are fully described, for example, in U.S. Patent Nos. 5,162,339, 5,232,929, 5,242,930, 5,373,003, 5,387,595, 5,459,270, 5,494,926, 5,496,833, 5,637,699, 5,719,147; European Patent Publication Nos. EP 0 360 390, 0 394 989, 0 428 434, 0 429 366, 0 430 771, 0 436 334, 0 443 132, 0 482 539, 0 498 069, 0 499 313, 0 512 901, 0 512 902, 0 514 273, 0 514 274, 0 514 275, 0 514 276, 0 515 681, 0 517 589, 0 520 555, 0 522 808, 0 528 495, 0 532 456, 0 533 280, 0 536 817, 0 545 478, 0 558 156, 0 577 394, 0 585 913,0 590 152, 0 599 538, 0 610 793, 0 634 402, 0 686 629, 0 693 489, 0 694 535, 0 699 655,

0 699 674, 0 707 006, 0 708 101, 0 709 375, 0 709 376, 0 714 891, 0 723 959, 0 733 632 and 0 776 893; PCT International Patent Publication Nos. WO 90/05525. 90/05729, 91/09844, 91/18899, 92/01688, 92/06079, 92/12151, 92/15585, 92/17449, 92/20661, 92/20676, 92/21677, 92/22569, 93/00330, 93/00331, 93/01159, 93/01165, 5 93/01169, 93/01170, 93/06099, 93/09116, 93/10073, 93/14084, 93/14113, 93/18023, 93/19064, 93/21155, 93/21181, 93/23380, 93/24465, 94/00440, 94/01402, 94/02461. 94/02595, 94/03429, 94/03445, 94/04494, 94/04496, 94/05625, 94/07843, 94/08997, 94/10165, 94/10167, 94/10168, 94/10170, 94/11368, 94/13639, 94/13663, 94/14767. 94/15903, 94/19320, 94/19323, 94/20500, 94/26735, 94/26740, 94/29309, 95/02595, 95/04040, 95/04042, 95/06645, 95/07886, 95/07908, 95/08549, 95/11880, 95/14017, 95/15311, 95/16679, 95/17382, 95/18124, 95/18129, 95/19344, 95/20575, 95/21819, 95/22525, 95/23798, 95/26338, 95/28418, 95/30674, 95/30687, 95/33744, 96/05181. 96/05193, 96/05203, 96/06094, 96/07649, 96/10562, 96/16939, 96/18643, 96/20197. 96/21661, 96/29304, 96/29317, 96/29326, 96/29328, 96/31214, 96/32385, 96/37489, 15 97/01553, 97/01554, 97/03066, 97/08144, 97/14671, 97/17362, 97/18206, 97/19084. 97/19942 and 97/21702; and in British Patent Publication Nos. 2 266 529, 2 268 931, 2 269 170, 2 269 590, 2 271 774, 2 292 144, 2 293 168, 2 293 169, and 2 302 689. The preparation of such compounds is fully described in the aforementioned patents and publications, which are incorporated herein by reference.

In an embodiment, the neurokinin-1 receptor antagonist for use in conjunction with the compounds of the present invention is selected from: 2-(R)-(1-(R)-(3,5-bis(trifluoromethyl)phenyl)ethoxy)-3-(S)-(4-fluorophenyl)-4-(3-(5-oxo-1H,4H-1,2,4-triazolo)methyl)morpholine, or a pharmaceutically acceptable salt thereof, which is described in U.S. Patent No. 5,719,147.

20

25

30

A compound designed or selected using the methods of the instant invention may also be administered with an agent useful in the treatment of anemia. Such an anemia treatment agent is, for example, a continuous eythropoiesis receptor activator (such as epoetin alfa).

A compound designed or selected using the methods of the instant invention may also be administered with an agent useful in the treatment of neutropenia. Such a neutropenia treatment agent is, for example, a hematopoietic growth factor which regulates the production and function of neutrophils such as a human granulocyte colony stimulating factor, (G-CSF). Examples of a G-CSF include filgrastim.

A compound designed or selected using the methods of the instant invention may also be administered with an immunologic-enhancing drug, such as levamisole, isoprinosine and Zadaxin.

Thus, the scope of the instant invention encompasses the use of the compounds designed or selected using the methods disclosed herein in combination with a second compound selected from:

5

25

30

19)

	_	
	1)	an estrogen receptor modulator,
	2)	an androgen receptor modulator,
•	3)	retinoid receptor modulator,
10	4)	a cytotoxic/cytostatic agent,
	5)	an antiproliferative agent,
	6)	a prenyl-protein transferase inhibitor,
	7)	an HMG-CoA reductase inhibitor,
	8)	an HIV protease inhibitor,
15	9)	a reverse transcriptase inhibitor,
	10)	an angiogenesis inhibitor,
	11)	a PPAR-γ agonists,
	12)	a PPAR-δ agonists,
	13)	an inhibitor of inherent multidrug resistance,
20	14)	an anti-emetic agent,
	· 15)	an agent useful in the treatment of anemia,
	16)	an agent useful in the treatment of neutropenia,
	17)	an immunologic-enhancing drug,
	18)	an inhibitor of cell proliferation and survival signaling, and

The term "administration" and variants thereof (e.g., "administering" a compound) in reference to a compound of the invention means introducing the compound or a prodrug of the compound into the system of the animal in need of treatment. When a compound of the invention or prodrug thereof is provided in combination with one or more other active agents (e.g., a cytotoxic agent, etc.), "administration" and its variants are each understood to include concurrent and sequential introduction of the compound or prodrug thereof and other agents.

an agent that interfers with a cell cycle checkpoint.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specified amounts, as well as any

product which results, directly or indirectly, from combination of the specified ingredients in the specified amounts.

The term "therapeutically effective amount" as used herein means that amount of active compound or pharmaceutical agent that elicits the biological or medicinal response in a tissue, system, animal or human that is being sought by a researcher, veterinarian, medical doctor or other clinician.

The term "treating cancer" or "treatment of cancer" refers to administration to a mammal afflicted with a cancerous condition and refers to an effect that alleviates the cancerous condition by killing the cancerous cells, but also to an effect that results in the inhibition of growth and/or metastasis of the cancer.

In an embodiment, the angiogenesis inhibitor to be used as the second compound is selected from a tyrosine kinase inhibitor, an inhibitor of epidermal-derived growth factor, an inhibitor of fibroblast-derived growth factor, an inhibitor of platelet derived growth factor, an MMP (matrix metalloprotease) inhibitor, an integrin blocker, interferon- α , interleukin-12, pentosan polysulfate, a cyclooxygenase inhibitor, carboxyamidotriazole, combretastatin A-4, squalamine, 6-O-chloroacetyl-carbonyl)-fumagillol, thalidomide, angiostatin, troponin-1, or an antibody to VEGF. In an embodiment, the estrogen receptor modulator is tamoxifen or raloxifene.

Also included in the scope of the claims is a method of treating cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with radiation therapy and/or in combination with a compound selected from:

- . 1) an estrogen receptor modulator,
- 2) an androgen receptor modulator,
- 25 a retinoid receptor modulator,

5

10 -

15

20

- 4) a cytotoxic/cytostatic agent,
- 5) an antiproliferative agent,
- 6) a prenyl-protein transferase inhibitor,
- 7) an HMG-CoA reductase inhibitor,
- 30 8) an HIV protease inhibitor,
 - 9) a reverse transcriptase inhibitor,
 - 10) an angiogenesis inhibitor,
 - 11) PPAR-y agonists,
 - 12) PPAR- δ agonists,
- an inhibitor of inherent multidrug resistance,

5

10

19)

14) an anti-emetic agent,
15) an agent useful in the treatment of anemia,
16) an agent useful in the treatment of neutropenia,
17) an immunologic-enhancing drug,
18) an inhibitor of cell proliferation and survival signaling, and

an agent that interfers with a cell cycle checkpoint.

And yet another embodiment of the invention is a method of treating cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with paclitaxel or trastuzumab.

The invention further encompasses a method of treating or preventing cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with a COX-2 inhibitor.

The instant invention also includes a pharmaceutical composition useful for treating or preventing cancer that comprises a therapeutically effective amount of a compound designed or selected using the methods disclosed herein and a compound selected from:

1) 2)	an estrogen receptor modulator, an androgen receptor modulator,
•	an androgen receptor modulator.
	,
. 3)	a retinoid receptor modulator,
· 4)	a cytotoxic/cytostatic agent,
.5)	an antiproliferative agent,
6)	a prenyl-protein transferase inhibitor,
7)	an HMG-CoA reductase inhibitor,
8)	an HIV protease inhibitor,
9)	a reverse transcriptase inhibitor,
10)	an angiogenesis inhibitor, and
11)	a PPAR-γ agonist,
12)	a PPAR-δ agonists;
13)	an inhibitor of cell proliferation and survival signaling, and
14)	an agent that interfers with a cell cycle checkpoint.
	5) 6) 7) 8) 9) 10) 11) 12) 13)

In each of the aforementioned uses of atomic coordinates of KSP, the coordinates according to Tables 1-4 are preferred.

Additional objects of the present invention will be apparent from the description which follows.

As used herein, the following terms and phrases shall have the meanings set forth below:

5

10

15

20

25

30

35

Unless otherwise noted, "KSP" includes both native and wild type Kinesin Spindle Protein as well as "KSP analogues", defined herein as proteins or peptides comprising a ligand binding site substantially as set forth in SEQ ID NO:1. Such KSP analogues include, but are not limited to, a ligand binding site characterized by a three-dimensional structure comprising the relative structural coordinates of amino acid residues set forth in Figure 10 as set forth in Tables 1-4, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 3.005 Å, more preferably not more than about 2.0Å, and most preferably not more than about 0.5 Å.

Unless otherwise indicated, "protein" or "molecule" shall include a protein, protein domain, polypeptide or peptide.

"Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using X-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three-dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original sets provided in Tables 1-4 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Tables 1-4.

An "agent", "ligand" or "binding partner" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound or drug.

"Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates

described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

5

MATERIALS AND METHODS

Materials and methods provided are intended to assist in a further understanding of the invention and are not to limit the reasonable scope thereof.

10

25

Motor Domain of Human KSP, Amino Acids 1-368
MASQPNSSAK KKEEKGKNIQ VVVRCRPFNL AERKASAHSI
VECDPVRKEV SVRTGGLADK SSRKTYTFDM VFGASTKQID
VYRSVVCPIL DEVIMGYNCT IFAYGQTGTG KTFTMEGERS

- 15 PNEEYTWEED PLAGIIPRTL HQIFEKLTDN GTEFSVKVSL
 LEIYNEELFD LLNPSSDVSE RLQMFDDPRN KRGVIIKGLE
 EITVHNKDEV YQILEKGAAK RTTAATLMNA YSSRSHSVFS
 VTIHMKETTI DGEELVKIGK LNLVDLAGSE NIGRSGAVDK
 RAREAGNINQ SLLTLGRVIT ALVERTPHVP YRESKLTRIL
- 20 QDSLGGRTRT SIIATISPAS LNLEETLSTL EYAHRAKNIL NKPEVNQK

Binding Pocket of Human KSP

Lining the newly formed pocket and surrounding the ligand are amino acid residues:

115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P) (from helix- α 2 and its insertion loop; residue 116 is at the end of the first portion of helix- α 2 and residue 134 is at the beginning of the second portion of helix- α 2 thus the insertion loop starts at residue 116

30 and ends at residue 134);

160(L) (from beta strain- β 4); 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) (from helix- α 3); and 239(F) (from beta strain- β 6).

35 KSP Expression

E. coli cells harboring the KSP (368 residues) vector were grown at 37°C in LB medium containing 100 μg/ml ampicillin. KSP expression was induced at 25°C with 0.5mM isopropyl-D (-)-thiogalactopyranoside, and the cells were grown for four additional hours at 25°C prior to harvest.

Cells from 10 litre were suspended in 75 ml lysis buffer (50mM PIPES, 2mM MgCl₂, 1mM ATP, 1mM TCEP, 1mM EGTA, protease inhibitor tablets (one tablet per 50ml buffer)) and homogenized. Cells were disrupted by passing the homogenized suspension thrice through 10 a Microfluidizer (Model 110-S). The cell lysate was centrifuged at 15,000 rpm for 30 minutes and the supernatant mixed with DE-52 resin (100 ml) pre-equilibrated in SP sepharose Buffer A (50mM PIPES, 2mM MgCl₂, 1mM ATP, 1mM TCEP, 1mM EGTA). Supernatant was removed after spinning at 1000 rpm for 10 minutes. Resin was washed twice with one resin 15 volume (100ml) of 50mM PIPES, 2mM MgCl₂, 1mM ATP, 1mM TCEP, 1mM EGTA. The supernatants were pooled and loaded onto SP sepharose column (50ml, 2.6cm diameter column, Amersham Biosciences). Kinesin with ~95% purity was eluted at 0.15 to 0.2 M KCl using 0-30% KCl gradient. The fractions containing KSP (by SDS-PAGE analysis) were 20 pooled and diluted with SP sepharose buffer A to a final KCl concentration of 50mM. The pool was mixed with 10ml of High performance Q-sepharose (Amersham Biosciencs) equilibrated in SP sepharose BufferA. The supernatent was collected by spinning at 1000rpm for 10 minutes. The resin was washed four times with two resin volume. The washes and supernatant 25 were pooled and concentrated on Centriprep-10 to 15 to 17mg/ml and stored in small alicots at -70° C. The protein was characterized by N-terminal sequence analysis by Edman degradation on an Applied Biosystem model 470A gas phase sequencer. Protein concentration was determined with quantitative amino acid analysis by using a post column ninhydrin 30 derivatization method on a Beckman 6300 analyzer. Molecular weight was determined on Deca-LCQ (Finnegan) mass spectrometer. Molar mass and size distribution was determined by multi-angle light scattering detector (Wyatt technology, DAWN EOS) connected to size exclusion column on Millenium HPLC.

5

Crystallization

5

30

The concentrated kinesin (ADP, Mg⁺⁺) protein at about 15mg/ml in 50mM PIPES buffer at pH 6.8 in the presence of 2mM MgCl₂, 1mM TECP, 1mM ATP, 84mM KCl, and 1mM EGTA was incubated with 1mM inhibitor Compound 5-2b ((+)-monastrol). Small single crystal seeds were obtained by hanging drop method with well solution containing 20% PEG3350, 0.15M K₂HPO₄ and 0.1M HEPES buffer at pH7.0 in about four days. Crystals suitable for X-ray data collection were obtained by macroseeding in hanging drops with well solution containing 14% PEG3350, 0.2M K₂HPO₄ and 0.1M HEPES at pH 6.8 in about two weeks. Hanging drops were formed by equal volume of protein and well solutions.

X-ray Data Collection and Procession

at 100K at synchrotron beamline 17-ID of the Advanced Photon Source at Argonne National Laboratory. Prior to data collection the crystal was soaked in the cryo-protectant solution for 20 minutes that contains 20% PEG3350, 0.15M K₂HPO₄, 20% PEG200, and 0.1M HEPES buffer at pH6.8. The crystal was then frozen in liquid nitrogen. The X-ray wavelength was set to 1Å. The data were collected at 0.2° oscillation per frame with 1000 frames total and 1 second exposure per frame at 250 mm detector to crystal distance. The data were processed and scaled by use of HKL2000 package. The crystal is in orthorhombic space group of P2₁2₁2₁ with cell dimensions of a= 69.5 Å b=79.5 Å and c=159.0 Å. The

Structure Determination and Refinement

The structure was determined by the use of the molecular replacement method in cooperation with extensive model rebuilding and dynamic refinement. The kinesin protein coordinates in the binary complex crystal structure of kinesin bound with ADP (Mg⁺⁺) was used as the search model. The molecular replacement solution was obtained with use of program AmoRe at 4.0Å to 15Å resolution range, which gave R-factor of 0.48 and correlation coefficient of 0.60. The initial protein model was

rebuilt and refined literally at 2.5Å resolution, those included dynamic refinement, energy minimization and temperature factor refinement. The Compound 5-2b density became apparent at the fourth rebuilding and refinement cycle. Finally, 441 water molecules were added in the model and the R-factor was 0.21 with R-free of 0.26 with good geometry (RMSD_{bonds} = 0.007 Å, RMSD_{angles} = 1.32°). The current protein model binds with one ADP, one Mg⁺⁺ ion and one Compound 5-2b. It starts at residue Asn18 to Lys362 with a gap from residue Asn271 to Asn287 (missing loop11 from Ile272 to Gly286) due to lack of electron density. There are two complexes in an asymmetric unit.

Tertiary Structure of KSP/ADP/Compound 5-2b

The 3-dimensional, tertiary structure of KSP, bound with Mg⁺⁺-ADP and Compound 5-2b ((+)-monastrol), was determined at 2.5Å resolution with use of phases derived from a combination of molecular replacement, extensive manual rebuilding, and dynamic refinement. Two identical protein complexes were found in the asymmetric unit of the crystal and were related by a local, non-crystallographic 2-fold axis. For each, the electron density of the protein as well as those of the ligands (ADP, Mg⁺⁺, and

20 Compound 5-2b) was all well defined. Compound 5-2b was seen to be of the S handedness. Residues 2-17, 272-286, and 363-368 were disordered and showed no electron densities (The N-terminal Met1 residue was processed upon expression). See Figures 1-8.

25 Fluorescence of Trp127 of KSP(368)-ADP -/+ Inhibitors

Materials

- -2X kinesin buffer: 160 mM K-Hepes, 2 mM MgCl₂, 2 mM EGTA, 2 mM DTT (added fresh daily), and 100 mM KCl, pH 6.8.
- -Nucleotide: nucleotide is resuspended to 200 mM in 50 mM K-Hepes (pH 6.8).
 - -Nucleotide is diluted 1:1 with 200 mM MgCl₂ to a stock concentration of 100 mM of 1:1 nucleotide:MgCl₂.
 - -Cuvette volume = 300 µl

Methods

1) Add 281 μ l of 1X kinesin buffer, \pm nucleotide, and H₂O (Nucleotide = none, 1 mM AMPPNP, or 1 mM ADP (final concentration)).

- 5 2) Add 18.75 μl of 4 μM stock nucleotide-free KSP(367H).
 - 3) Add compound sequentially from DMSO stock (with all the volume of all additions $\leq 0.6 \,\mu$ l).
 - 4) Measure fluorescence after each addition (starting with buffer only).
- Example titration for Compound 8-1 with KSP(367H)ADP:
 281 μl of 1X kinesin buffer + 1 mM ADP:
 add 250 nM KSP (18.75 μl of 4 uM nucleotide-free stock)
 add 1 nM Compound 8-1 (1 nM_f) (addition of 0.3 μl of 0.001 mM stock)
 add 2 nM Compound 8-1 (3 nM_f) (addition of 0.6 μl of 0.001 mM stock)
- add 4 nM Compound 8-1 (7 nM_f) (addition of 0.12 μl of 0.01 mM stock) add 3 nM Compound 8-1 (10 nM_f) (addition of 0.09 μl of 0.01 mM stock) add 20 nM Compound 8-1 (30 nM_f) (addition of 0.6 μl of 0.01 mM stock) add 40 nM Compound 8-1 (70 nM_f) (addition of 0.12 μl of 0.1 mM stock) add 30 nM Compound 8-1 (100 nM_f) (addition of 0.09 μl of 0.1 mM stock)
- add 200 nM Compound 8-1 (300 nM_f) (addition of 0.6 μl of 0.1 mM stock) add 400 nM Compound 8-1 (700 nM_f) (addition of 0.12 μl of 1 mM stock) add 300 nM Compound 8-1 (1000 nM_f) (addition of 0.09 μl of 1 mM stock) add 2000 nM Compound 8-1 (3000 nM_f) (addition of 0.6 μl of 1 mM stock).
 - 6) After each addition, measure steady-state fluorescence under the following conditions:

 $\lambda_{ex} = 388$ nm, $\lambda_{em} = 342-346$ nm, band width = 3 nm ex/3 nm em, wavelength increment = 0.5 nm, integration time = 2 s.

7) Repeat the same titration series:
in the absence of KSP (to determine compound-related background), and
in the absence of KSP, but in the presence of 1 µM L-tryptophan (to
determine compound-related effects on the amino acid itself).

Calculations

25

At the peak emission wavelength for W127 in KSP(367H) (=344 nm) measure the compound emission in kinesin buffer as a function of [compound]; measure fluorescence of L-tryptophan as a function of [compound]; measure fluorescence of KSP(367H) as a function of [compound]; correct KSP(367H) fluorescence for its decrease over time (due to losses of protein to the cuvette); subtract compound emission from L-tryptophan emission; subtract compound emission from KSP(367H) emission. Calculate the fraction of fluorescence of L-tryptophan vs [compound]: (L-trp fluorescence (344 nm) at given [compound]) / (L-trp fluorescence (344 nm) at given [compound]) / (KSP fluorescence (344 nm) at given [compound]) / (KSP fluorescence (344 nm) at 0 cpd); then normalize: KSP (frcn fl) / L-trp(frcn fl) and plot vs [compound].

Results of this assay are illustrated in Figures 11-13.

15

Compounds that were utilized in the identification and testing of the novel KSP binding site that is disclosed herein may be prepared by the methods described below:

SCHEME 1

5 <u>Step 1</u>: 3-[3-(benzyloxy)phenyl]-1-(2-chlorophenyl)prop-2-en-1-one (1-4)

10

To a solution of 2'-chloroacetophenone (1-1) (1.26mL, 9.70mmol) in 40 mL of THF at -78°C was slowly added 10.7 mL (10.7mmol) of a 1M LiHMDS solution in THF. After stirring for 1h at -78°C, a solution of 2.05g (9.70mmol) of 3-benzyloxy-benzaldehyde (1-2) in

8 mL of THF was added, and stirring was continued at that temperature for an additional hour. The mixture was then dumped into a separatory funnel containing 100 mL of saturated aqueous NH4Cl and extracted twice with 100 mL of EtOAc. The organic phases were combined, washed with 100 mL of brine, and dried over Na₂SO₄. After filtering off the drying agent, the solvent was removed on a rotary evaporator, and the residue was dissolved in 50 mL of CH₂Cl₂. After cooling to -78°C, 4 mL of triethylamine and 2 mL of trifluoroacetic anhydride were added sequentially, and the mixture was allowed to warm to rt and stir for 12h. The reaction was then dumped into a separatory funnel with 100 mL of 1M HCl, the layers were separated, and the aqueous phase extracted again with CH2Cl2. The organic layers were combined, washed again with 1 M HCl, washed with water, and dried over Na₂SO₄. After concentration, the crude material was purified by chromatography on silica gel with a gradient of 0 to 40% EtOAc in hexanes over 45 min to provide <u>1-4</u> as a viscous yellow oil. Data for <u>1-4</u>: ¹HNMR $(500 \text{ MHz}, \text{CDCl}_3) \delta 7.5 - 7.0 \text{ (m, 15H) } 5.1 \text{ (s, 2H) ppm.}$

5

15

35

Step 2: 1-(2-chlorophenyl)-3-(hydroxyphenyl)prop-2-en-1-one (1-5)

To a solution of 740 mg (2.12mmol) of 1-4 in 15 mL of

20 CH₂Cl₂ at -78°C was added dropwise 2.75 mL (2.75mmol) of a 1M solution of BBr₃ in CH₂Cl₂. After stirring for 30 min at that temperature, 1 mL of MeOH was added, and the mixture was dumped into water, extracted twice with 50 mL of CH₂Cl₂, washed again with water, and dried over Na₂SO₄. After concentration, the residue was purified by column chromatography on silica gel with a gradient of 2 to 70% EtOAc in hexanes over 30 min to provide 1-5 as a beige solid. Data for 1-5: ¹HNMR (500 MHz, CDCl₃) δ 7.5 - 7.3 (m, 5H), 7.25 (m, 1H), 7.2 - 7.0 (m, 3H), 6.9 (m, 1H), 5.1 (bs, 1H) ppm.

30 Step 3: 3-[1-acetyl-3-(2-chlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl]phenol (1-7)

To a solution of 120mg (0.46mmol) of chalcone $\underline{1-5}$ in 4 mL of acetic acid was added 50 μ L (0.93mmol) of hydrazine hydrate. The reaction was then placed in an oil bath at 110°C for 24h. After cooling to rt, the solvents were removed on a rotary evaporator, the residue was dissolved

in 50 mL of CH₂Cl₂, washed twice with aqueous NaHCO₃, dried over Na₂SO₄, and concentrated. The residue was then purified by column chromatography on silica gel with a gradient of 5 to 75% EtOAc in hexanes over 30 min to provide $\underline{1-7}$ as a fluffy white solid. Data for $\underline{1-7}$: ¹HNMR (500 MHz, CDCl₃) δ 7.75 (m, 1H), 7.45 (m 1H), 7.4 – 7.3 (m, 2H), 7.2 (m,

5

1H), 6.8 (d, 1H), 6.7 (m, 2H), 5.5 (m, 1H), 3.9 (m, 1H), 3.3 (m, 1H), 2.4 (s, 3H) ppm. HRMS (ES) calc'd M + H for $C_{17}H_{15}ClN_2O_2$: 315.0895. Found: 315.0904.

SCHEME 2

Step 1: 2,5-difluorobenzenediazonium tetrafluoroborate (2-1)

5

15

20

25

30

35

Nitrosonium tetrafluoroborate (905 mg, 7.75 mmol, 1.00 equiv) was added to a solution of 2,5-difluoroaniline (0.780 mL, 7.75 mmol, 1 equiv) in acetonitrile (50 mL) at 0°C. The resulting mixture was stirred for 1 h, then diluted with ethyl ether (150 mL). The precipitate was filtered and air-dried to give 2,5-difluorobenzenediazonium tetrafluoroborate (2-1) as a tan solid. 1 H NMR (300 MHz, CD₃OD) δ 8.54 (m, 1H), 8.24 (m, 1H), 7.95 (m, 1H).

10 <u>Step 2</u>: tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (2-2)

Palladium(II) acetate (67 mg, 0.30 mmol, 0.020 equiv) was added to a vigourously stirred, deoxygenated mixture of tert-butyl 2,5dihydro-1H-pyrrole-1-carboxylate (2.59 mL, 15.0 mmol, 1 equiv) and 2,5difluorobenzenediazonium tetrafluoroborate (2-1, 3.42 g, 15.0 mmol, 1.00 equiv) in water and carbon tetrachloride (1:1, 150 mL) at 23°C, and the resulting mixture was stirred for 20 h. The reaction mixture was concentrated, and the residue partitioned between ethyl acetate (300 mL) and saturated aqueous sodium bicarbonate solution (75 mL). The organic layer was washed with brine, then dried over sodium sulfate and concentrated. The residue was dissolved in toluene (200 mL), and the resulting solution concentrated in vacuo to facilitate azeotropic removal of residual water. 2,6-Lutidine (3.50 mL, 30.0 mmol, 2.00 equiv) and trifluoroacetic anhydride (1.48 mL, 10.5 mmol, 0.700 equiv) were then sequentially added to a solution of the residue in toluene (100 mL) at -10°C. The resulting mixture was allowed to warm to 10 °C over 16 h, then heated at reflux for 1 h. The reaction mixture was allowed to cool to 23°C, then concentrated. The residue was partitioned between ethyl acetate (300 mL) and saturated aqueous sodium bicarbonate solution (150 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by flash column chromatography (hexanes initially, grading to 20% EtOAc in hexanes) to give tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1carboxylate (2-2) as a red oil. ¹H NMR (500 MHz, CDCl₃) major rotamer; δ 7.03-6.84 (m, 3H), 6.70 (br s, 1H), 5.01 (br s, 1H), 4.42 (m, 1H), 4.13 (m, 1H), 3.60 (m, 1H), 1.50 (s, 9H).

Step 3: tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4)

5

10

15

20

25

30

35

Tris(dibenzylideneacetone)dipalladium(0) (59 mg, 064 mmol, 0.020 equiv) was added to a deoxygenated mixture of tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (2-2, 900 mg, 3.20 mmol, 1 equiv), benzenediazonium tetrafluoroborate (1-3, prepared by the method described above for 2-3, 614 mg, 3.20 mmol, 1.00 equiv), and sodium acetate trihydrate (1.32 g, 9.60 mmol, 3.00 equiv) in acetonitrile (70 mL) at 23°C. The reaction mixture was stirred for 16 h, then partitioned between saturated aqueous sodium bicarbonate solution and ethyl acetate (2 x 70 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column chromatography (hexanes initially, grading to 40% hexanes in EtOAc) to provide tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4) as an orange oil. LRMS m/z (M+H-CH₃) 343.0 found, 343.1 required.

Step 4: 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5)

Trifluoroacetic acid (20 mL) was added to a solution of tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4, 700 mg, 1.96 mmol, 1 equiv) in dichloromethane (50 mL) at 23 °C, and the resulting mixture was stirred for 30 min, then concentrated to give 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5) as a TFA salt (brown oil). LRMS m/z (M+H) 258.1 found, 258.1 required.

<u>Step 5</u>: 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-<u>1H-pyrrole-1-carboxamide (2-6)</u>

Triethylamine (1.37 mL, 9.79 mmol, 5.00 equiv) and dimethylcarbamoyl chloride (0.180 mL, 1.96 mmol, 1.00 equiv) were added to a solution of 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5, 1.96 mmol) in dichloromethane (50 mL) at 23°C, and the resulting mixture was stirred for 2 h, then concentrated. The residue was partitioned between saturated aqueous sodium bicarbonate solution (75 ml) and ethyl acetate (100 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by reverse-phase LC (H₂O/CH₃CN

gradient w/ 0.1 % TFA present) to provide 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6) as an off-white solid. 1 H NMR (500 MHz, CDCl₃) δ 7.35-7.29 (m, 4H), 7.25 (m, 1H), 7.05 (m, 1H), 7.00 (m, 1H), 6.96 (m, 1H), 6.40 (br s, 1H), 6.13 (m, 1H), 4.88 (ddd, 1H, J = 13.7, 5.6, 2.0 Hz), 4.52 (d, 1H, J = 13.7 Hz), 2.88 (s, 6H). LRMS m/z (M+H) 329.1 found, 329.1 required.

5

10

<u>Step 6</u>: Enantiomers of 4-(2,5-difluorophenyl)-N,N-dimethyl-2-<u>phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-7 and 2-8)</u> Resolution of enantiomers of racemic 4-(2,5-difluorophenyl)-

N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6) by chiral normal-phase HPLC (Chiralcel OD column: 0.1 % diethylamine in 40% ethanol in hexanes) provided in order of elution 2-7 (-) and 2-8 (+).

SCHEME 3

5

Step 1: (2S,4S)-tert-Butyl 4-hydroxy-2-phenylpyrrolidine-1-carboxylate (3-2)

To a flame dried flask equipped with stir bar was added tertbutyl (2S,4S)-4-{[tert-butyl(dimethyl)silyl]oxy}-2-phenylpyrrolidine-1carboxylate (3-1, prepared from (S)-(-)-4-chloro-3-hydroxybutyronotrile by 5 the method of Maeda, et al Synlett 2001, 1808-1810, 7.8 g, 20.7 mmol) and anhydrous acetonitrile (20.0 mL). The resulting solution was treated with triethylamine trihydrofluoride (10.1 mL, 62.0 mmol) while stirring under N₂. The reaction stirred 12 h at 40 °C. The reaction was then diluted with EtOAc 10 (100 mL) and poured into 5% aq. NaHCO₃. Following cessation of gas evolution, the organic layer was washed three addition times with 5% aq. NaHCO₃. The organic layer was dried over magnesium sulfate, filtered and concentrated to provide crude product. Recrystallization was effected from EtOAc/hexanes to provide (2S,4S)-tert-butyl 4-hydroxy-2phenylpyrrolidine-1-carboxylate (3-2) as a white crystalline solid. ¹H NMR 15 (300 MHz, CDCl₃) rotamers δ 7.38-7.18 (m, 5H), 4.90 (m, 1H), 4.42 (m, 1H), 3.88 (m, 1H), 3.56 (dd, J = 11.5, 4.0 Hz, 1H), 2.60 (m, 1H), 2.03 (m, 1H), 1.50 and 1.20 (br s, 9H); MS 208.0 found, 208.1 (M – C(CH₃)₃)

20

25

30

35

required.

Step 2: (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3–3)

To a flame dried flask equipped with stir bar was added 150 mL anhydrous dichloromethane which was cooled to -78 °C. Oxalyl chloride (3.8 mL, 44 mmol) and DMSO (4.8 mL, 61 mmol) were added sequentially and the reaction stirred for 10 min. (2S,4S)-tert-butyl 4-hydroxy-2-phenylpyrrolidine-1-carboxylate (3-2, 2.28 g, 8.73 mmol) in 10 mL anhydrous dichloromethane was added dropwise and stirred 1 h at -78°C. Triethylamine (12 mL, 87mmol) was added and the reaction was warmed to 0°C over 1 h. Upon completion, the reaction was washed with 5% NaHCO₃, brine and dried over MgSO₄. The organic layer was concentrated to provide crude (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3-3). Recrystallization was effected with EtOAc/hexanes. ¹H NMR (300 MHz, CDCl₃) δ 7.35 (m, 3H), 7.17 (m, 2H), 5.38 (m, 1H), 4.08 (d, *J* = 19.5 Hz, 1H), 3.90 (d, *J* = 19.3 Hz, 1H), 3.13 (dd, *J* = 18.8, 9.8 Hz,

1H), 2.58 (dd, J = 18.6, 2.4 Hz, 1H), 1.40 (br s, 9H); MS 206.0 found, 206.1 (M – C(CH₃)₃) required.

Step 3: (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}2,5-dihydro-1H-pyrrole-1-carboxylate (3-4)

5

10

15

20

25

30

To a flame dried flask equipped with stir bar was added ketone (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3-3, 0.16 g, 0.62 mmol) and anhydrous THF (2 mL). The resulting solution was cooled to -78 °C, and treated dropwise with lithium hexamethyldisilylamide (LHMDS, 0.68 mL, 1M in THF, 0.68 mmoL). The reaction stirred 1 h at -78 °C, and N-(5-chloropyridin-2-yl)-1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-methanesulfonamide (0.27 g, 068 mmol) was added neat in one portion. The reaction was allowed to warm to 0 °C and stirred 4 hours total. The reaction was diluted with Et2O (10mL) and washed successively with H₂O (10mL) and brine (10 mL). The organic layer was dried over MgSO₄, filtered and concentrated. The crude residue was purified by flash column choromatography (0-20% EtOAc/hexanes gradient, 15 min) to provide (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5dihydro-1H-pyrrole-1-carboxylate (3-4). ¹H NMR (300 MHz, CDCl₃) major rotamer: δ 7.30 (m, 5H), 5.72 (m, 1H), 5.48 (m, 1H), 4.42 (m, 2H), 1.18 (s, 9H); MS 379.0 found 379.1 (M - CH₃) required.

Step 4: (2S)-4-(2,5-difluorophenyl)-2-phenyl-N,N-dimethyl-2,5-dihydro-1H-pyrrole-1-carboxamide (3-5)

To a flame dried flask equipped with stir bar was added (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5-dihydro-1H-pyrrole-1-carboxylate (3–4, 0.250 g, 0.636 mmol), 2,5-difluorophenyl boronic acid (0.251 g, 1.59 mmol), Na₂CO₃ (0.202 g, 1.91 mmol), and LiCl (0.081 g, 1.91 mmol). The solids were dissolved in 20 mL 4:1 DME/H₂O and degassed with nitrogen. Pd(PPh₃)₄ (0.037 g, 0.032 mmol) was added and the reaction was sealed under nitrogen and heated to 90 °C for 2 h. Upon completion, the reaction was partitioned between 5% aq. NaHCO₃ and EtOAc (3 x 50 mL), and the combined organic layers were dried over MgSO₄. Following filtration, the organic layer was concentrated and

purified via flash column chromatography (SiO₂, 0-20% EtOAc/hexanes gradient) to provide (2S)-tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (3-5). Further transformations followed those described in Scheme 1 to provide the instant compound 2-6.

5

15

20

SCHEME 4

H 1. CHO

H₂SO₄,

NH₂ H₂O/EtOH

2. MeNCO, acetone

$$\frac{4-2a \text{ (Trans)}}{4-2b \text{ (Cis)}}$$

10 Trans-1H-Imidazo[1',5':1,6]pyrido[3,4-b]indole-1,3(2H)-dione,5,6,11,11a-tetrahydro-2-methyl-5-(3-hydroxyphenyl) (4-2a)

To a mixture of DL-tryptophan (1.5 g, 7.44 mmol), 3-hydroxybenzaldehyde (0.90, 7.44 mmol) in EtOH (3 mL) was added aq. H₂SO₄ (14.9 mL of a 0.5 M solution). The reaction was heated to 50 C for 12 h. The reaction mixture was partly concentrated to remove EtOH and resuspended in H₂O (5 mL). The precipitate was collected by filtration and dried in vacuo. The portion of this solid residue (0.14 g, 0.47 mmol) was dissolved in acetone (3 mL) and treated with methyl isocyanate. The reaction mixture was heated at 150 C in a sealed vessel for 15 min in a microwave reactor. The reaction was cooled to r.t. and concentrated. The residue was absorbed onto silica gel then purified on an ISCO automated system affixed with a Biotage flash 40(s) cartridge eluting with 0-100% EtOAc in hexane at 20 mL/min over 30 min to afford a mixture of 4-2a/4-2b Trituration of this mixture with diethyl

ether provided pure 4-2a. Data for 4-2a: 1 HNMR (600 MHz, CD₃OD) δ 7.52 (d, J = 8 hz, 1H), 7.27 (d, J = 8 hz, 1H), 7.18 (m, 1H), 7.12 (m, 1H), 7.07 (m, 1H), 6.84 (m, 1H), 6.74 (m, 2H), 6.24 (s, 1H), 4.44 (m, 1H), 3.43 (m, 1H), 3.01 (s, 3H), 2.88 (m, 1H) ppm. HRMS Calcd (M+1) 348.1270; found 348.1343.

SCHEME 5

10

5

(-)4-(3-Hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-4H-pyrimidin-5-carboxylic acid ethyl ester (5-2a) and (+)-4-(3-Hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-4H-pyrimidin-5-carboxylic acid ethyl ester (5-2b)

15

20

Racemic monastrol (50 mg, Tocris) was resolved by chiral HPLC (Chiralpak AD column 5 x 50 cm; 20% EtOH/80% (hexanes + 0.1% diethylamine); flow = 60 mL/min) to yield (-)-enantiomer $\underline{1\text{-}2A}$ (R_T =57.0 min) and (+)-enantiomer $\underline{5\text{-}2B}$ (R_T = 71.2 min). Enantiomer $\underline{5\text{-}2B}$ was crystallized from hexanes to yield a yellow solid.

SCHEME 6

SCHEME 6 (continued)

5

10

SCHEME 6 (continued)

$$\begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

tert-Butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2)

A solution of tert-butyllithium in pentane (1.7 M, 42.5 mL, 72.3 mmol, 2.40 equiv) was added to a solution of tert-butyl thien-2-ylcarbamate (6-1, 6.00 g, 30.1 mmol, 1 equiv) in THF (300 mL) at -78 °C. The reaction mixture was stirred for 45 min, then solid CO₂ (approximately 20 g) was added and the resulting mixture was warmed to 0 °C and stirred for 30 minutes. The reaction mixture was partitioned between aqueous 1 N hydrochloric acid solution and ethyl acetate (2 x 150 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue

was purified by flash column chromatography (hexanes initially, grading to 100% ethyl acetate), and the polar fractions were concentrated. A solution of the residue, benzylamine (6.61 g, 61.7 mmol, 2.05 equiv), 1-(3dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (5.91 g, 30.8 5 mmol, 1.02 equiv), 1-hydroxy-7-azabenzotriazole (4.19 g, 30.8 mmol, 1.02 equiv), and triethylamine (8.59 mL, 61.7 mmol, 2.05 equiv) in DMF (100 mL) was stirred at 55°C for 24 h. The reaction mixture was concentrated, and the residue was partitioned between saturated aqueous sodium bicarbonate solution and ethyl acetate (3 x 100 mL). The combined organic 10 layers were dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to give tert-butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2) as a colorless oil. ¹H NMR (300 MHz, CDCl₃) δ 7.37 (m, 5H), 6.87 (d, 1H, J =5.8 Hz), 6.69 (d, 1H, J = 5.8 Hz), 6.13 (s, 1H), 4.61 (d, 2H, J = 5.5 Hz), 1.52 15 (s, 9H).

N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3)

A solution of tert-butyl 3-[(benzylamino)carbonyl]thien-2ylcarbamate (6-2, 500 mg, 1.50 mmol, 1 equiv) was saturated with HCl gas 20 at 0 °C, and the resulting solution was stirred at 0 °C for 1 h, then allowed to warm to 23 °C and stirred for 1 h. The reaction mixture was concentrated and the residue was dissolved in pyridine (10 mL). The resulting solution was cooled to 0 °C, and butyryl chloride (420 μL, 4.04 mmol, 2.69 equiv) was added in three equal portions over 1 h. The reaction mixture was 25 partitioned between aqueous sodium bicarbonate solution and ethyl acetate (50 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to give N-benzyl-2-(butyrylamino)thiophene-3carboxamide (6-3) as an off-white solid. ¹H NMR (300 MHz, CDCl₃) δ 7.36 30 (m, 5H), 6.92 (d, 1H, J = 6.1 Hz), 6.76 (d, 1H, J = 5.8 Hz), 6.23 (s, 1H), 4.62 (d, 2H, J = 5.8 Hz), 2.47 (t, 2H, J = 7.3 Hz), 1.80 (sextet, 2H, J = 7.3Hz), 1.01 (t, 3H, J = 7.3 Hz).

3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4)

5

10

A mixture of N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3, 230 mg, 0.76 mmol, 1 equiv) and sodium hydroxide (3 mg, 0.08 mmol, 0.1 equiv) in ethylene glycol (5 mL) was heated at 130 °C for 5 h. The reaction mixture was allowed to cool, then partitioned between a half-saturated aqueous sodium chloride solution and ethyl acetate (2 x 75 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to provide 3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4) as a colorless oil which solidified upon standing. ¹H NMR (300 MHz, CDCl₃) δ 7.48 (d, 1H, J = 5.8 Hz), 7.31 (m, 3H), 7.19 (d, 1H, J = 5.8 Hz), 7.17 (d, 2H, J = 7.9 Hz), 5.42 (s, 2H), 2.72 (t, 2H, J = 7.6 Hz), 1.78 (sextet, 2H, J = 7.6 Hz), 0.97 (t, 3H, J = 7.3 Hz).

3-benzyl-5,6-dibromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-5) and 3-benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-6)

A solution of 3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4, 100 mg, 0.35 mmol, 1 equiv), potassium acetate (207 mg, 20 2.1 mmol, 6 equiv) and bromine (338 mg, 2.1 mmol, 6 equiv) in acetic acid (2 mL) was heated at 100°C for 3 hr. The reaction was concentrated, and the residue was purified by flash chromatography. Elution with 30 % hexanes/EtOAc gave 3-benzyl-5,6-dibromo-2-(1-bromopropyl)thieno[2,3d]pyrimidin-4(3H)-one (6-5) as a colorless solid. ¹H NMR (500 MHz, 25 CDCl₃) δ 7.30 (m, 1H), 7.14 (d, J = 7.3 Hz, 2H), 6.19 (d, J = 16.3 Hz, 1H). 4.87 (d, J = 16.3 Hz, 1H), 4.62 (t, J = 7.3 Hz, 1H), 2.35 (m, 1H), 2.18 (m, J= 1H), 0.72 (t, J = 7.3 Hz, 3H). Further elution with the same eluant gave 3benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (2-6) as a colorless gum. ¹H NMR (500 MHz, CDCl₃) δ 7.53 (s, 1H), 7.34 (m, 30 2H), 7.29 (m, 1H), 7.12 (d, J = 7.3 Hz, 2H), 6.21 (d, J = 16.3 Hz, 1 H), 4.88 (d, J = 16.3 Hz, 1H), 4.62 (t, J = 7.2 Hz, 1H), 2.37 (m, 1H), 2.18 (m, 1H),0.72 (t, J = 7.3 Hz, 3H).

3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-7)

A solution of 3-benzyl-5,6-dibromo-2-(1-

5

10

15

20

25

30

35

bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-5, 35 mg, 0.066 mmol, 1 equiv) and N,N-dimethylethylenediamine (17 mg, 0.198 mmol, 3 equiv) in ethanol (5mL) was heated at reflux for 18 h. The reaction was concentrated, and the residue was partitioned between EtOAc and brine. The organic layer was dried (MgSO₄) and concentrated to provide 3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno-[2,3-d]pyrimidin-4(3H)-one (6-7) as a yellow gum. MS(M+1) = 526.8.

3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8)

A solution of 3-benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-6, 35 mg, 0.079 mmol, 1 equiv) and N,N-dimethylethylenediamine (21 mg, 0.237 mmol, 3 equiv) in ethanol (5mL) was heated at reflux for 18 h. The reaction was concentrated, and the residue was partitioned between EtOAc and brine. The organic layer was dried (MgSO₄) and concentrated to provide 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}-propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8) as a yellow gum. MS(M+1) = 449.9.

N-[1-(3-benzyl-5,6-dibromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-9)

A solution of 4-bromobenzoyl chloride (19 mg, 0.085 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8, 45 mg, 0.085 mmol, 1 equiv) and N,N-diisopropylethylamine (11 mg, 0.085 mmol, 1 equiv) in dichloromethane (5 mL), and the resulting reaction mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous NaHCO₃ solution, then brine, and dried (MgSO₄) and concentrated. The residue was purified by reverse-phase LC (H₂O/CH₃CN gradient w/ 0.1 % TFA present) to provide N-[1-(3-benzyl-5,6-dibromo-4-oxo-3,4-dihydrothieno[2,3-

d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-9) as a colorless foam. MS(M+1) = 708.9

N-[1-(3-benzyl-6-bromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-10)

5

A solution of 4-bromobenzoyl chloride (19 mg, 0.085 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-9, 38 mg, 0.085 mmol, 1 equiv) and N,N-

- diisopropylethylamine (11 mg, 0.085 mmol, 1 equiv) in dichloromethane (5 mL), and the resulting reaction mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous NaHCO₃ solution, and brine, then dried (MgSO₄) and concentrated. The residue was purified by reverse-phase LC (H₂O/CH₃CN gradient w/ 0.1 % TFA present)
- to provide N-[1-(3-benzyl-6-bromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-10) as a colorless foam. 1 H NMR (500 MHz, CDCl₃) δ 7.55 (m, 3H), 7.31 (m, 5H), 7.14 (m, 2H), 6.04 (d, J = 15.4 Hz, 1H), 5.92 (m, 1H), 5.12 (d, J = 15.4 Hz, 1H), 3.37 (m, 2H), 2.05 (m, 4 H), 1.83 (m, 6H), 0.65 (m, 3H).

10

SCHEME 7

5 3-benzyl-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1)

A mixture of 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]-amino}propyl)-thieno[2,3-d]pyrimidin-4(3H)-one (6-8,17 mg, 0.38 mmol, 1 equiv) and 10 % Pd/C in ethyl acetate (5 mL) was hydrogenated at 1 atm. for 3 h. The mixture was filtered and the filtrate concentrated to provide 3-benzyl-2-(1-{[2-

(dimethylamino)ethyl]amino)propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1) as a pale yellow gum. MS(M+1) = 371.1.

N-[1-(3-benzyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (7-2)

.5

10

15

20

A solution of 4-bromobenzoyl chloride (8 mg, 0.035 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1, 13 mg, 0.035 mmol, 1 equiv) and N,N-diisopropylethylamine (5 mg, 0.035 mmol, 1 equiv) in dichloromethane (1 mL), and the resulting mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous NaHCO₃ solution, and brine, then dried (MgSO₄) and concentrated. The residue was purified by flash chromatography. Elution with CH₂Cl₂ to 5 % NH₃-EtOH/CH₂Cl₂ gave N-[1-(3-benzyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (7-2) as an off-white foam. ¹H NMR (500 MHz, CDCl₃) δ 7.31 (m, 5H), 7.14 (m, 2H), 6.09 (d, J = 15.6 Hz, 1H), 5.94 (m, 1H), 5.10 (d, J = 15.6 Hz, 1H), 3.40 (m, 2H), 2.11 (m, 1H), 2.03 (m, 2H), 1.87 (m, 1H), 1.79 (s, 6H), 0.66 (t, J = 6.6 Hz, 3H).

SCHEME 8

3-benzyl-2-(1-{(4-bromobenzyl)[2-

(t, J = 7 Hz, 3H).

(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one(8-1)
A solution of 3-benzyl-2-(1-{[2-

Ś (dimethylamino)ethyl]amino}-propyl)thieno[2,3-d]pyrimidin-4(3H)-one(7-1, 175 mg, 0.47 mmol, 1 equiv) and 4-bromobenzaldehyde (174 mg, 0.94 mmol, 2 equiv) in methanol (20 mL) was treated with a solution of sodium cyanoborohydride in tetrahydrofuran (1 M, 0.94 mL, 0.94 mmol, 2 equiv). Acetic acid was added to obtain a pH of 6-7 and the reaction was warmed at 10 60 °C for 18 h. An additional 2 equivalents of 4-bromobenzaldehyde and sodium cyanoborohydride were added after 18, 42 and 66 hours while maintaining the pH at 6-7 with acetic acid. After warming 90 h at 60°C, the reaction was concentrated and the residue was partitioned between EtOAc and aqueous saturated NaHCO₃ solution. The organic layer was washed with brine, dried (MgSO₄) and concentrated. The residue was purified by flash 15 chromatography. Elution with EtOAc to 5 % NH3-EtOH/EtOAC gave 3benzyl-2-(1-{(4-bromobenzyl)[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one(8-1) as a pale yellow gum. ¹H NMR (500 MHz, CDCl₃) δ 7.45 (d, J = 6 Hz, 1H), 20 7.33 (d, J = 8 Hz, 2H), 7.21 (m, 4H), 7.05 (d, J = 8 Hz, 2H), 6.84 (d, J = 7H2, 2H), 5.85 (d, J = 16 Hz, 1H), 5.32 (d, J = 16 Hz, 1H), 3.87 (d, J = 14Hz, 1H), 3.73 (dd, J = 11, 3 Hz, 1H), 3.50 (d, J = 14 Hz, 1H), 2.92 (m, 1H), 2.61 (m, 1H), 2.28 (m, 2H), 2.15 (m, 1H), 2.07 (s, 6H), 1.74 (m, 1H), 0.64

TABLE 1

```
REMARK complex 1 with water molecules surrounding it
       REMARK r= 0.2114 free r= 0.2639
REMARK rmsd bonds= 0.006712 rmsd angles= 1.32262
 5
       REMARK B rmsd for bonded mainchain atoms= 1.570
REMARK B rmsd for bonded sidechain atoms= 2.570
                                                               target= 1.5
       REMARK B rmsd for bonded sidechain atoms=
                                                               target= 2.0
       REMARK B rmsd for angle mainchain atoms= 2.729 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.936 target= 2.5
10
       REMARK sg- P2(1)2(1)2(1) a= 69.48 b= 79.54 c= 158.98 alpha= 90. beta= 90. gamma= 90.
       REMARK reflection file= k2a.cv
       REMARK B-correction resolution: 6.0 - 2.5
       REMARK FILENAME="kin_16dpb.pdb"
       MOTA
                     CB ASN
                                           37.472
                                                    -7.942 100.393
                                                                      1.00 28.28
                                  18
                                                                                         Α
15
       ATOM
                     CG
                         ASN
                                           38.236
                                                    -7.260 101.506
                                                                      1.00 31.25
                                  18
                                                                                         Α
                     OD1 ASN
                                           38.752
                                                    -7.913 102.413
       ATOM
                                  18
                                                                      1.00 36.19
                                                                                         A
       MOTA
                     ND2 ASN
                                  18
                                           38.310
                                                    -5.940 101.448
                                                                      1.00 32.46
       ATOM
                          ASN
                                           35.178
                                                    -7.311 101.124
                                                                      1.00
                                                                            24.09
       ATOM
                          ASN
                                           34.900
                                                    -6.997 102.284
                                                                      1.00 23.76
20
       MOTA
                     N
                          ASN
                                  18
                                           35.576
                                                    -9.454
                                                            99.859
                                                                      1.00
       ATOM
                  R
                     CA
                          ASN
                                  18
                                           36.124
                                                    -8.484 100.856
                                                                      1.00 25.50
       ATOM
                  9
                     N
                          ILE
                                  19
                                           34.708
                                                    -6.636 100.074
                                                                      1.00
                                                                            21.79
                                                    -5.540 100.278
-4.791 98.970
       MOTA
                 10
                     CA
                         ILE
                                  19
                                           33.759
                                                                      1.00 19.48
       ATOM
                 11
                     CB
                         ILE
                                  19
                                           33.425
                                                                      1.00 20.49
25
                     CG2 ILE
                                                    -3.992
       ATOM
                                  19
                                           32.124
34.573
                 12
                                                             99.129
                                                                      1.00 19.87
                     CG1 ILE
                                                             98.613
       ATOM
                 13
                                  19
                                                    -3.846
                                                                      1.00
                                                                            20.82
       ATOM
                     CD1 ILE
                                  19
                                           34.194
                 14
                                                    -2.801
                                                             97.563
                                                                      1.00 19.23
                                           32.487
                                                    -6.185 100.820
       ATOM
                 15
                                  19
                     С
                          ILE
                                                                      1.00 18.08
                                                    -7.079 100.190
       ATOM
                 16
                     0
                          ILE
                                  19
                                           31.929
                                                                      1.00 17.25
30
                                                    -5.743 101.991
       ATOM
                 17
                          GLN
                                  20
                                           32.044
                                                                      1.00 16.72
       MOTA
                 18
                     CA
                          GLN
                                  20
                                           30.863
                                                    -6.315 102.624
                                                                      1.00 17.94
       ATOM
                     ÇВ
                          GLN
                                           30.996
                                                    -6.207 104.143
                                                                      1.00 18.71
       MOTA
                 20
                     CG
                          GLN
                                  20
                                           32.221
                                                    -6.950 104.689
                                                                      1.00 19.97
       ATOM
                 21
                      CD
                          GLN
                                  20
                                           32.369
                                                    -6.829 106.196
                                                                      1.00 21.29
35
       MOTA
                 22
                     OE1 GLN
                                  20
                                           32.511
                                                    -5.730 106.734
                                                                      1.00
                                                                            22.63
       MOTA
                 23
                     NE2 GLN
                                  20
                                           32.336
                                                    -7.964 106.885
                                                                      1.00 22.16
       MOTA
                 24
                     C
                          GLN
                                  20
                                           29.560
                                                    -5.681 102.147
                                                                      1.00 17.78
       ATOM
                 25
                     0
                          GLN
                                  20
                                           29.396
                                                    -4.462 102.184
                                                                      1.00 -19.12
                                                    -6.528 101.695
                                                                      1.00 14.78
       MOTA
                 26
                     N
                          VAL
                                  21
                                           28.640
40
                                                    -6.080 101.176
-6.609 99.738
                 27
                                  21
21
                          VAL
                                           27.355
27.144
       ATOM
                     CA
                                                                      1.00 13.75
                 28
                          VAL
       MOTA
                     CB
                                                                      1.00 14.14
                                                                                         Α
                                                    -6.065
-6.238
                                                             99.155
       ATOM
                 29
                     CG1 VAL
                                  21
                                           25.854
                                                                      1.00 11.78
                 30
                     CG2 VAL
                                  21
       ATOM
                                                             98.875
                                                                      1.00 13.09
                                           28.339
                                                                                         Α
                          VAL
                                  21
                                                    -6.571 102.036
       ATOM
                 31
                     C
                                           26.198
                                                                      1.00 14.04
45
                                  21
                                                    -7.756 102.365
       MOTA
                 32
                     0
                          VAL
                                           26.128
                                                                      1.00 13.35
       MOTA
                 33
                          VAL
                                  22
                                           25.294
                                                    -5.659 102.396
                                                    -6.011 103.194
       ATOM
                 34
                     CA.
                          VAL
                                           24.123
                                                                      1.00
                                                                            14.01
       ATOM
                 35
                     CB
                          VAL
                                           24.197
                                                    -5.423 104.627
                                                                      1.00 15.50
       MOTA
                 36
                     CG1 VAL
                                  22
                                           25.588
                                                    -5.628 105.201
                                                                      1.00 16.80
50
       MOTA
                 37
                     CG2 VAL
                                  22
                                           23.817
                                                    -3.968 104.623
                                                                      1.00
                                                                            15.97
                                                                      1.00 13.29
       MOTA
                 38
                     С
                          VAL
                                  22
                                           22.838
                                                    -5.518 102.532
       MOTA
                 39
                     0
                          VAL
                                  22
                                           22.811
                                                    -4.469 101.884
                                                                      1.00
                                                                            13.40
       MOTA
                 40
                     N
                          VAL
                                  23
                                           21.773
                                                    -6:292 102.694
                                                                      1.00 12.04
                                                    -5.953 102.125
       MOTA
                 41
                     CA
                          VAL
                                  23
                                           20.478
                                                                      1.00 11.16
                                                    -7.155 101.350
-6.883 100.979
55
                                  23
23
       MOTA
                 42
                          VAL
                     CB
                                           19.890
                                                                      1.00 10.39
                 43
                         VAL
       ATOM
                     CG1
                                           18.423
                                                                      1.00
                                                                             6.97
                                                                                         Α
                     CG2
                                  23
                                                    -7.429 100.112
       ATOM
                         VAL
                 44
                                           20.733
                                                                             5.75
                                                                      1.00
                                  23
                 45
      ATOM
                          VAL
                                           19.496
                                                    -5.551 103.220
                     С
                                                                      1.00 12.26
                                                                                         Α
                                           19.433
18.734
                                  23
       ATOM
                 46
                          VAL
                                                    -6.180 104.276
                     0
                                                                      1.00 12.72
60
                                                    -4.497 102.965
                 47
                          ARG
                                  24
       ATOM
                     N
                                                                      1.00
                                                                            12.29
       MOTA
                 48
                     CA
                          ARG
                                  24
                                           17.741
                                                    -4.033 103.925
                                                                      1.00 11.98
                                  24
       MOTA
                 49
                     СВ
                          ARG
                                           18.150
                                                    -2.711 104.572
                                                                             9.94
                                                                      1.00
       ATOM
                 50
                     CG
                          ARG
                                  24
                                           17.092
                                                    -2.197 105.533
                                                                             9.40
                                                                      1.00
       MOTA
                 51
                     CD
                          ARG
                                           17.412
                                                    -0.826 106.110
                                                                      1.00 11.24
65
                 52
       ATOM
                     NE
                          ARG
                                           16.638
                                                    -0.585 107.326
                                                                      1.00
                                                                             8.87
       MOTA
                 53
                          ARG
                                           16.668
                                                     0.540 108.033
                                                                      1.00
                                                                            11.40
       MOTA
                 54
                     NH1
                          ARG
                                                     1.563 107.649
                                           17.432
                                                                      1.00 11.52
                                                     0.629 109.151
       ATOM
                 55
                     NH2 ARG
                                  24
                                           15.956
                                                                      1.00 12.63
       ATOM
                 56
                     С
                          ARG
                                  24
                                           16.404
                                                    -3.831 103.230
                                                                      1.00
                                                                            13.62
70
       MOTA
                 57
                     0
                          ARG
                                  24
                                           16.248
                                                    -2.918 102.415
                                                                      1.00 14.61
       MOTA
                 58
                     N
                          CYS
                                  25
                                           15.446
                                                    -4.690 103.553
                                                                      1.00 12.77
```

	MOTA	59	CA	CYS	25	14.117	-4.599	102.983	1.00 13.88	A
	MOTA	60	CB	CYS	25	13.461	-5.980	102.951	1.00 15.60	A
	ATOM	61	SG	CYS	25	11.855		102.134	1.00 21.58	Ä
		62								
5	MOTA		C	CYS	25	13.292		103.865	1.00 13.78	A
,	MOTA	63	0	CYS	25	13.293		105.084	1.00 15.62	A
	MOTA	64	N	ARG	26	12.605	-2.713	103.261	1.00 12.12	A
	MOTA	65	CA	ARG	26	11.774	-1.815	104.045	1.00 12.61	A
	MOTA	66	CB	ARG	26	11.601		103.343	1.00 10.76	A
	ATOM	67	CG	ARG	26	10.679		102.128		
10									1.00 7.66	A
10	MOTA	68	CD	ARG	26	10.181		101.775	1.00 7.16	A
	MOTA	69	NE	ARG	26	9.592	0.934	100.442	1.00 7.55	A
	MOTA	70	CZ	ARG	26	8.413	0.411	100.125	1.00 8.80	A
	ATOM	71	NH1	ARG	26	7.677	-0.194	101.052	1.00 8.81	A
	MOTA	72		ARG	26	7.980	0.472	98.876	1.00 7.02	A
15	MOTA	73	c	ARG						
1 5						10.407		104.215	1.00 15.65	A
	MOTA	74	0	ARG	26	10.058		103.500	1.00 17.10	. А
	MOTA	75	N	PRO	27	9.615	-1.982	105.170	1.00 17.31	A
	MOTA	76	CD	PRO	27	9.957	-1.053	106.262	1.00 18.01	A
	MOTA	77	CA	PRO	27	8:287	-2.562	105.382	1.00 20.54	A
20	ATOM	78	CB	PRO	27	8.037		106.858	1.00 19.92	A
	ATOM	79	CG	PRO	27	8.639				
								107.017	1.00 17.88	A
	ATOM	80	C	PRO	27	7.237		104.492	1.00 23.41	A
	MOTA	81	0	PRO	27	7.482	-0.833	103.916	1.00 23.28	A
~ -	MOTA	82	N	PHE	28	6.080	-2.542	104.371	1.00 26.52	A
25	MOTA	83	CA	PHE	28	4.976		103.584	1.00 29.18	A
	ATOM	84	СВ	PHE	28	3.805		103.588	1.00 27.65	
	ATOM	85		PHE						
					28	3.948		102.610	1.00 28.35	A
	MOTA	86	CD1		28	3.947		103.045	1.00 28.03	A
20	MOTA	87	CD2		28	4.038	-3.850	101.243	1.00 27.68	A
30	MOTA	88	CE1	PHE	28	4.026	-6.477	102.139	1.00 27.56	A
	MOTA	89	CE2	PHE	28	4.119	-4.893	100.324	1.00 29.26	A
	ATOM	90	CZ	PHE	28	4.112		100.773	1.00 27.81	A
	ATOM	91	c	PHE	28					
						4.513		104.191	1.00 32.56	A
35	ATOM.	92	0	PHE	28	4.426		105.411	1.00 33.43	A
22	MOTA	93	N	ASN	29	4.217	0.299	103.345	1.00 37.21	Α .
	MOTA	94	CA	ASN	29	3.744	1.595	103.829	1.00 42.32	A
	MOTA	95	CB	ASN	29	4.073	2.692	102.809	1.00 42.04	A
	ATOM	96	CG	ASN	29	3.604		101.410	1.00 41.31	Ä
	MOTA	97	OD1							
40					29	2.409		101.168	1.00 41.82	À
40	MOTA	98	ND2		29	4.546		100.482	1.00 40.11	A
	MOTA	99	С	ASN	29	2.232	1.526	104.054	1.00 46.51	A
	MOTA	100	0	ASN	29	1.606	0.505	103.768	1.00 46.59	A
	ATOM	101	N	LEU	30	1.650	2.612	104.562	1.00 51.19	A
	MOTA	102	CA	LEU	30	0.212		104.826	1.00 54.81	A.
45	ATOM	103	CB	LEU	30	-0.178				
								105.362	1.00 56.40	A
	ATOM	104	CG	LEU	30	-1.659		105.705	1.00 58.19	A
	MOTA	105	CD1		30	-2.058	3.273	106.820	1.00 57.83	A
	MOTA	106	CD2	LEU	30	-1.899	5.680	106.130	1.00 59.11	A
	ATOM	107	С	LEU	30	-0.637	2.343	103.592	1.00 56.70	A
50	ATOM	108	0	LEU	30	-1.552		103.658	1.00 56.66	A
	ATOM	109	N	ALA	31	-0.329		102.471	1.00 59.03	A
	ATOM	110	CA	ALA	31	-1.062		101.222	1.00 61.19	
										A
	ATOM	111	CB	ALA	31	-0.414		100.100	1.00 61.28	A
<i>E E</i>	MOTA	112	С	ALA	31	-1.125	1.316	100.833	1.00 62.78	A
55	MOTA	113	0	ALA	31	-2.123	0.850	100.282	1.00 62.16	A
	MOTA	114	N	GLU	32	-0.048	0.593	101.117	1.00 65.22	A
	MOTA	115	CA	GĻU	32		-0.827		1.00 67.27	A
	ATOM	116		GLU	32	1.501		100.702		
									1.00 66.96	A
60	MOTA	117	CG	GLU	32	2.199	-0.712	99.453	1.00 67.12	A
UU	MOTA	118	CD	GLU	32	3.713	-0.641	99.590	1.00 67.26	A
	MOTA	119	OE1	GLU	32	4.392	-0.422	98.563	1.00 66.83	A
	MOTA	120	OE2	GLU	32	4.223		100.723	1.00 65.99	A
	ATOM	121	С	GLU	32	-0.706		101.844	1.00 68.26	Ä
	ATOM	122	ŏ	GLU	32	-1.260				
65								101.526	1.00 68.16	· A
55	ATOM	123	N	ARG	33	-0.722		103.087	1.00 69.65	A
	MOTA	124	CA	ARG	33	-1.403		104.169	1.00 71.22	A
	ATOM	125	CB .	ARG	33	-1.196	-1.162	105.498	1.00 72.33	A
	MOTA	126	CG .	ARG	33	0.239	-1.138	106.009	1.00 73.65	A
	MOTA	127	CD	ARG	33	0.695		106.479	1.00 74.57	A
70	MOTA	128	NE	ARG	33	2.043		107.041	1.00 76.44	Ä
	MOTA	129	cz	ARG	33					
						2.692		107.521	1.00 76.91	A
	MOTA	130	NH1		33	2.119		107.513	1.00 76.68	A
	MOTA	131	NH2	ARG	33	3.918	-3.376	108.007	1.00 77.35	A

			_							
•	MOTA	132	C	ARG	33	-2.901		103.885	1.00 71.74	A
	MOTA MOTA	133 134	O N	ARG LYS	33 34	-3.464 -3.536		103.900 103.632	1.00 71.46 1.00 71.80	A
	MOTA	135	CA	LYS	34	-4.967		103.032	1.00 71.67	A A
5	ATOM	136	СВ	LYS	34	-5.426		103.195	1.00 72.94	A
_	ATOM	137	ÇG	LYS	34	-4.734		102.072	1.00 74.72	A
	MOTA	138	CD	LYS	34	-5.218		101.986	1.00 75.69	À
	ATOM	139	CE	LYS	34	-6.680	2.936	101.565	1.00 75.79	A
10	MOTA	140	NZ	LYS	34	-7.149	4.343	101.426	1.00 74.45	A
10	MOTA	141	C	LYS	34	-5.315		102.088	1.00 70.68	A
	ATOM	142	.0	LYS	34	-6.448		101.924	1.00 70.80	A
	ATOM	143	N	ALA	35	-4.338		101.198	1.00 68.59	A
•	MOTA	144	CA	ALA	35 35	-4.539	-2.501	99.963	1.00 66.37	A
15	MOTA MOTA	145 146	CB C	ALA ALA	35 35	-3.639	-1.949	98.861 100.241	1.00 65.65	A
15	MOTA	147	ŏ	ALA	35	-4.199 -4.277	-4.807	99.352	1.00 64.89 1.00 64.01	A A
	ATOM	148	N	SER	36	-3.825		101.491	1.00 63.72	Ä
	ATOM	149	CA	SER	36	-3.454		101.937	1.00 62.31	Ä
	ATOM	150	СВ	SER	36	-4.711		102.194	1.00 62.73	A
20	MOTA	151	OG	SER	36	-5.556	-6.469	101.056	1.00 63.14	A
	MOTA	152	С	SER	36	-2.542		100.920	1.00 60.52	A
	ATOM	153	0	SER	36	-2.933		100.256	1.00 60.52	Α.
	MOTA	154	N	ALA	37	-1.316		100.818	1.00 57.81	A
25	MOTA	155	CA	ALA	37	-0.339	-6.291	99.877	1.00 54.58	'A
23	MOTA MOTA	156 157	CB C	ALA ALA	37 37	0.709	-5.228	99.561	1.00 53.39	A
	ATOM	158	ò	ALA	37	0.351 0.586		100.359	1.00 51.84 1.00 50.84	A
	ATOM	159	N	HIS	38	0.669	-8.429	99.405	1.00 48.60	A A
	MOTA	160	CA	HIS	38	1.363	-9.672	99.690	1.00 45.12	A
30	MOTA	161	СB	HIS	38		-10.810	98.840	1.00 48.05	A
	MOTA	162	CG	HIS	38	0.753	-10.528	97.364	1.00 50.18	A
	ATOM	163	CD2	HIS	38	-0.262	-10.171	96.542	1.00 51.32	A
	MOTA	164		HIS	38		-10.621	96.566	1.00 50.53	A
35	MOTA	165		HIS	38		-10:337	95.317	1.00 50.82	A
22	MOTA MOTA	166		HIS	38		-10.059	95.275	1.00 51.95	Α
•	ATOM	167 168	0	HIS	38 38	2.836 3.165	-9.436 -9.005	99.350 98.244	1.00 40.69	A
	MOTA	169	N	SER	39			100.312	1.00 39.51	A A
	ATOM	170	CA	SER	39	5.138		100.106	1.00 29.81	A
40	ATOM	171	CB	SER	39	5.860		101.449	1.00 29.59	A
	MOTA	172	OG	SER	39	7.263		101.265	1.00 30.93	A
	ATOM	173	С	SER	39		-10.578	99.242	1.00 27.18	A
	ATOM	174	0	SER	39	5.507	-11.758	99.456	1.00 27.84	A
45	MOTA	175	N	ILE	40		-10.179	98.263	1.00 23.70	A
45	ATOM ATOM	176 177	CA CB	ILE	40		-11.148	97.403	1.00 20.93	A
	MOTA	178	CG2	ILE	40 40		-10.677 -10.554	95.945 95.381	1.00 21.59 1.00 21.07	A
	MOTA	179	CG1		40	8.025	-9.343	95.857	1.00 21.07	A A
	ATOM	180	CD1		40	8.377	-8.954	94.443	1.00 17.86	A
50	ATOM	181	C	ILE	40		-11.366	97.895	1.00 19.29	Ä
	MOTA	182	0	ILE	40		-12.130	97.306	1.00 18.82	A
	ATOM	183	N	VAL	41 .	8.987	-10.696	98.988	1.00 18.43	A
	ATOM	184	CA	VAL	41		-10.801	99.572	1.00 19.01	A
55	ATOM	185	CB	VAL	41	10.974	-9.394	99.666	1.00 18.10	A
22	MOTA	186	CG1		41	12.231		100.525	1.00 17.03	A
	MOTA MOTA	187 188	CG2		41 41	11.303	-8.881	98.279 100.976	1.00 16.81	A
	MOTA	189	0	VAL	41		-11.420		1.00 21.10 1.00 22.16	A A
	ATOM	190	N	GLU	42		-12.286		1.00 21.96	A
60 -	ATOM	191	CA	GLU	42			102.595	1.00 24.43	Â
	MOTA	192	СВ	GLU	42		-14.310		1.00 26.41	A
	ATOM	193	CG	GLU	42		-14.321		1.00 33.53	A
	MOTA	194	CD	GLU	42	8.646	-15.717	102.435	1.00 37.53	A
65	MOTA	195	OE1		42		-15.830		1.00 37.91	A
65	ATOM	196	OE2		42		-16.695		1.00 39.48	A
	MOTA	197	C	GLU	42		-12.912		1.00 23.06	A
	MOTA	198	O N	GLU	42		-13.313		1.00 23.11	A
	ATOM ATOM	199 200	N CA	CYS	43 43		-12.461		1.00 22.56	A
70	ATOM	201	CB	CYS	43		-12.417 -11.032		1.00 22.27 1.00 21.27	A A
. •	ATOM	202		CYS	43	14.515		103.330	1.00 26.40	A A
	ATOM	203		CYS	43		-13.458		1.00 23.32	A
	MOTA	204	0	CYS	43		-13.850		1.00 25.24	A

	MOTA	205	N	ASP	44	15.936	-13.900	105.909	1.00 24.35	A
	ATOM	206	CA	ASP	44			106.873	1.00 24.49	Ä
	ATOM	207	СВ	ASP	44			106.182	1.00 24.72	A
~	MOTA	208	CG	ASP	.44	16.638	-17.408	107.164	1.00 27.03	A
5	MOTA	209		ASP	44	17.089	-17.201	108.313	1.00 28.16	A
	ATOM .	210	OD2	ASP	44			106.780	1.00 27.08	A
	MOTA	211	С	ASP	44			107.404	1.00 24.36	A
	MOTA	212	0	ASP	44			106.923	1.00 23.06	A
10	MOTA	213	N	PRO	45			108.411	1.00 25.65	A
10	MOTA	214	CD	PRO	45			109.059	1.00 25.98	A
	MOTA MOTA	215 216	CA CB	PRO PRO	45 45			108.971	1.00 26.11	Α
	ATOM	217	CG	PRO	45			110.133 109.657	1.00 25.67 1.00 26.57	A
	ATOM	218	C	PRO	45			109.637	1.00 26.95	A A
15	ATOM	219	ŏ	PRO	45			109.111	1.00 26.64	Ä
	ATOM	220	N	VAL	46			110.140	1.00 27.42	Ä
	MOTA	221	CA	VAL	46			110.636	1.00 28.91	À
	MOTA	222	CB	VAL	46			111.522	1.00 28.55	A
20	ATOM	223	CG1	VAL	46	18.882	-18.096	110.655	1.00 28.05	A
20	MOTA	224	CG2	VAL	46			112.465	1.00 28.65	A
	ATOM	225	C	VAL	46			109.506	1.00 30.17	A
	ATOM	226	0	VAL	46			109.688	1.00 29.93	A
	ATOM	227	N	ARG	47			108.333	1.00 30.73	A
25	ATOM ATOM	228 229	CA CB	ARG	47 47			107.195	1.00 31.90	A
23	ATOM	230	CG	ARG	47			106.515 107.286	1.00 35.93 1.00 43.15	· A
	ATOM	231	CD	ARG	47			106.799	1.00 48.31	· A
	ATOM	232	NE	ARG	47			105.352	1.00 52.94	Ä
	ATOM	233	CZ	ARG	47			104.697	1.00 53.97	A
30	MOTA	234	NH1	ARG	47			105.356	1.00 54.33	A
	ATOM	235		ARG	47	17.773	-21.561	103.381	1.00 54.58	A
	MOTA	236	C	ARG	47			106.171	1.00 30.25	A
	ATOM	237	0	ARG	47			105.122	1.00 27.99	A
35	ATOM ATOM	238	N	LYS	48			106.484	1.00 29.50	A
55	MOTA	239 240	CA CB	LYS LYS	48 48			105.586	1.00 28.39 1.00 28.24	A
	MOTA	241	CG	LYS	48			105.423	1.00 28.24	A A
	MOTA	242	CD	LYS	48			107.677	1.00 23.13	A
	ATOM	243	CE	LYS	48			108.651	1.00 34.18	Ä
40	ATOM	244	NZ	LYS	48			107.950	1.00 34.16	A
	MOTA	245	С	LYS	48	21.564	-14.415	104.209	1.00 27.13	A
	ATOM	246	0	LYS	48			103.188	1.00 27.94	A
	ATOM	247	N	GLU	49			104.170	1.00 25.69	A
45	MOTA MOTA	248 249	CA CB	GLU	49 49			102.895	1.00 26.19	Α
1.5	MOTA	250	CG	GLU	49			102.827	1.00 28.94 1.00 34.48	A A
	ATOM	251	CD	GLU	49			101.710	1.00 39.36	Ä
	ATOM	252		GLU	49			102.067	1.00 40.10	Ä
~^	ATOM	253	OE2	GLU	49			101.516	1.00 39.93	A
50	MOTA	254	С	GLU	49		-14.113	102.607	1.00 24:38	A
	MOTA	255	0	GLU	49			103.496	1.00 24.72	A
	ATOM	256	N	VAL	50			101.349	1.00 22.04	A
	ATOM ATOM	257 258	CA CB	VAL VAL	50 50			100.928	1.00 21.18	A
55	ATOM	259		VAL	50		-11.619	100.410 99.127	1.00 21.63 1.00 21.68	A
	ATOM	260		VAL	50			100.190	1.00 21.00	A A
	ATOM	261		VAL	. 50			99.821	1.00 19.98	Ä
	ATOM	262	o	VAL	50		-14.282	98.912	1.00 20.15	A
	ATOM	263	N	SER	51	15.087	-14.074	99.917	1.00 21.09	A
60	MOTA	264	CA	SER	51		-14.890	98.934	1.00 21.32	A
	MOTA	265	CB	SER	51		-16.106	99.629	1.00 20.35	A
	ATOM	266	OG	SER	51		-16.943	98.712	1.00 23.49	A
	MOTA	267	C	SER	51		-14.067	98.256	1.00 20.53	Α
65	ATOM ATOM	268 269	O N	SER	51 52		-13.401	98.925	1.00 21.64	.A
-	ATOM	270	N CA	VAL VAL	52		-14.107 -13.348	96.929 96.189	1.00 21.28	A
	MOTA	271	ÇВ	VAL	52		-12.293	95.282	1.00 22.46 1.00 21.66	A A
	ATOM	272	CG1		52		-11.462	94.605	1.00 21.60	A
70	MOTA	273	CG2		52		-11.417	96.091	1.00 19.80	A
70	MOTA	274	С	VAL	52	11.336	-14.220	95.322	1.00 24.82	A
	MOTA	275	0	VAL	52		-15.099	94.597	1.00 26.25	A
	MOTA	276	N	ARG	53 53		-13.964	95.409	1.00 27.28	A
	MOTA	277	CA	ARG	53	9.034	-14.690	94.638	1.00 29.70	A

	MOTA	278	СВ	ARG	53		-14.562	95.341	1.00 29.44	A
	ATOM ATOM	279 280	CG	ARG	53 53		-15.238 -15.124	94.658	1.00 32.62	A
	MOTA	281	CD NE	ARG	53		-15.124	95.536 96.805	1.00 32.33 1.00 34.30	A A
5	MOTA	282	cz	ARG	53		-15.618	97.894	1.00 35.73	Ä
_	ATOM	283	NH1		53		-14.743	97.877	1.00 35.26	Ä
	MOTA	284			53		-16.297	99.001	1.00 33.24	Ä
	ATOM	285	С	ARG	53	8.992	-14.062	93.243	1.00 30.22	A
10	MOTA	286	0	ARG	53	8.554	-12.922	93.080	1.00 28.70	A
10	ATOM	287	N	THR	54		-14.809	92.244	1.00 32.13	A
	MOTA	288	CA	THR	54		-14.314	90.872	1.00 35.09	A
	MOTA	289	CB	THR	54		-14.788	90.153	1.00 34.03	A
•	ATOM	290		THR	54		-16.218	90.086	1.00 33.22	A
15	ATOM	291	CG2	THR	54		-14.305	90.898	1.00 33.36	A
13	ATOM ATOM	292 293	C O	THR THR	54 54		-14.705 -14.098	90.011 88.970	1.00 38.38 1.00 39.08	A
•	MOTA	294	N	GLY	55		-15.717	90.435	1.00 39.08	A A
	ATOM	295	CA	GLY	55		-16.145	89.653	1.00 47.68	Ä
	ATOM	296	c.	GLY	55		-15.562	90.171	1.00 52.55	A
20	ATOM	297	õ	GLY	55		-14.562	89.651	1.00 52.62	A
	ATOM	298	N	GLY	56		-16.196	91.204	1.00 56.07	A
	ATOM	299	CA	GLY	56	3.343	-15.734	91.789	1.00 58.64	Α,
	MOTA	300	С	GLY	56		-16.804	92.620	1.00 60.65	A
25	MOTA	301	0	GLY	56		-17.999	92.444	1.00 60.57	A
25	MOTA	302	N	LEU	57		-16.364	93.532	1.00 62.43	A
	MOTA	303	CA	LEU	57		-17.253	94.421	1.00 63.41	A
	MOTA MOTA	304 305	CB CG	LEU	57 _. 57	-0.466	-18.425	93.627	1.00 63.91	A
	ATOM	306		LEU	57		-19.486	92.419 91.873	1.00 64.67 1.00 64.88	A A
30	ATOM	307		LEU	57	-1.654		92.806	1.00 64.92	A.
•	ATOM	308	c	LEU	5 <i>7</i>		-17.800	95.586	1.00 63.25	Ä
	ATOM	309	ō	LEU	57		-18.393	95.383	1.00 63.31	A
•	MOTA	310	N	ALA	58		-17.591	96.807	1.00 62.63	A
25.	MOTA	311	CA	ALA	58		-18:074	98.010	1.00 61.38	Α
35 1	MOTA	· 312	CB	ALA	58		-17.286	99.229	1.00 60.84	A
	MOTA	313	C	ALA	58		-19.562	98.184	1.00 60.68	A
	ATOM	314	0	ALA	58		-20.261	98.979	1.00 60.38	A
	MOTA	315	N	ASP	. 59		-20.024	97.422	1.00 59.38	A
40	MOTA MOTA	316 317	CA CB	ASP ASP	59 59 .		-21.413 -21.498	97.427 96.770	1.00 57.30 1.00 58.25	A
70	ATOM	318	CG	ASP	59 .	-1.438		96.386	1.00 58.25	A A
	MOTA	319		ASP	59		-23.767	97.285	1.00 58.25	A
	MOTA	320		ASP	59		-23.151	95.175	1.00 59.46	A
	MOTA	321	С	ASP	59		-22.267	96.652	1.00 55.60	A
45	MOTA	322	0	ASP	59	1.588	-23.414	97.007	1.00 55.05	A
	MOTA	323	N	LYS	60		-21.681	95.587	1.00 53.85	A
	MOTA	324	CA	LYS	60		-22.340	94.718	1.00 51.83	A
	ATOM	325	CB	LYS	60		-23.322	93.787	1.00 52.01	A
50	MOTA	326	CG	LYS	60		-23.940	92.720	1.00 51.22	A
50	ATOM ATOM	· 327 328	CD	LYS LYS	60 60		-24.835 -25.341	91.795 90.663	1.00 50.89 1.00 52.06	A A
	MOTA	329	NZ	LYS	60		-24.213	89.891	1.00 52.67	A
	MOTA	330	c	LYS	60		-21.258	93.900	1.00 50.64	Ä
	ATOM	331	ŏ	LYS	60		-20.350	93.358	1.00 51.26	A
55	MOTA	332	N	SER	61		-21.347	93.805	1.00 46.71	A
	MOTA	333	CA	SER	61	5.582	-20.340	93.056	1.00 42.61	A
	MOTA	334	CB	SER	61	5.478	-18.996	93.778	1.00 42.79	A
	MOTA	335	OG	SER	61		-19.048	95.039	1.00 41.39	Α
κ٥ .	MOTA	336	C	SER	61		-20.668	92.846	1.00 40.50	A
60	MOTA	337	0	SER	61		-21.619	93.412	1.00 39.84	A
	MOTA	338	N	SER	62		-19.856	92.017	1.00 37.70	A
	ATOM ATOM	339 340	CA CB	SER SER	62 62		-19.99B -19.776	91.732 90.245	1.00 34.42 1.00 34.68	A
	ATOM	341	OG	SER	62	10.742		89.964	1.00 34.68	A A
65	MOTA	342	C	SER	62		-18.917	92.554	1.00 32.09	A
	ATOM	343	ŏ	SER	62		-17.903	92.888	1.00 32.03	Ä
	ATOM	344	N	ARG	63	11.062		92.896	1.00 30.00	Ā
	ATOM	345	CA	ARG	63	11.775		93.690	1.00 29.48	A
70	MOTA	346	CB	ARG	63	11.685		95.189	1.00 31.57	A
70	MOTA	347	CG	ARG	63	10.273		95.710	1.00 35.27	A
	MOTA	348	CD	ARG	63	10.178		97.218	1.00 37.21	A
	MOTA	349	NE.	ARG	63	10.260		97.590	1.00 42.67	Α
	ATOM	350	CZ	ARG	63	9.885	-16.601	98.768	1.00 44.05	Α

	MOTA	351	MH1	ARG	63	9 995	-15.299	99.014	1.00 42.72	A
	MOTA	352	NH2		63		-17.408	99.700	1.00 46.01	A
	ATOM	353	C.	ARG	63	13.239	-17.994	93.314	1.00 27.46	A
	ATOM	354	0	ARG	63		-18.887	92.702	1.00 26.59	A
5										
,	MOTA	355	N	LYS	64		-16.853	93.693	1.00 25.59	A
	ATOM	356	CA-	LYS	64	15.216	-16.539	93.467	1.00 23.77	Ą
	ATOM	357	СВ	LYS	64	15 353	~15.299	92.587	1.00 25.43	À
	MOTA	358	CG	LYS	64	15.991	-15.532	91.231	1.00 26.32	A
	MOTA	359	CD	LYS	64	15.095	-16.338	90.323	1.00 28.26	A
10										
10	ATOM'	360	CE	LYS	64		-16.456	88.925	1.00 29.50	A
	MOTA	361	NZ .	LYS	64	15.825	-15.135	88.250	1.00 27.38	A
	ATOM	362	С	LYS	64	15.808	-16.257	94.854	1.00 23.10	A
		363	ō		64					
	MOTA			LYS			-15.488	95.637	1.00 22.42	A
	MOTA	364	N	THR	65	16.943	-16.876	95.154	1.00 22.03	A
15	MOTA	365	CA	THR	65 .	17.586	-16.715	96.452	1.00 20.67	A
		366		THR	65		-18.081	97.179		
	MOTA		CB						1.00 21.12	A
	MOTA	367	OG1	THR	65	16.352	-18.252	97.870	1.00 22.06	A
	MOTA	368	CG2	THR	65	18.740	-18.187	98.154	1.00 27.20	A
							-16.136			
20	ATOM	369	C	THR	65			96.363	1.00 19.65	A
20	ATOM	370	0	THR	65	19.735	-16.430	95.425	1.00 22.34	A
	MOTA	371	N	TYR	66	19.377	-15.300	97.331	1.00 17.01	A
	MOTA	372	CA	TYR	66		~14.695		1.00 15.46	
										A
	MOTA	373	CB	TYR	66	20.686	-13.244	96.829	1.00 14.31	A
	MOTA	374	CG	TYR	66	20.034	-13.055	95.482	1.00 14.28	A
25	ATOM	375		TYR	66		-12.984	95.366	1.00 12.32	- A
23										
	MOTA	376	CE1	TYR	66	18.046	-12.799	94.130	1.00 14.42	. A
	MOTA	377	CD2	TYR	66	20.804	-12.938	94.320	1.00 12.69	A
	ATOM	378		TYR	66		-12.752	93.079	1.00 10.53	A
20	MOTA	379	CZ	TYR	66	18.829	-12.682	92.993	1.00 13.34	. А
30	MOTA	380	OH	TYR	66	18.214	-12.483	91.776	1.00 14.95	A
	MOTA	381	С	TYR	66		-14.675	98.754	1.00 14.50	A
	MOTA	382	0	TYR	66	20.580	-14.461	99.733	1.00 13.73	A
	ATOM	383	N	THR	67.	22.605	-14.880	98.854	1.00 14.35	A
	MOTA	384	CA	THR	67		-14.853		1.00 15.82	A
35										
JJ	MOTA	385	CB	THR	67		-16.127		1.00 16.72	Α -
	MOTA	386	OG1	THR	67	23.209	-17.261	100.418	1.00 17.16	A
	MOTA	387	CG2	THR	67		-16.045		1.00 17.80	A
	MOTA	388	С	THR	67		-13.650		1.00 16.72	A
	MOTA	389	0	THR	67	24.992	-13.450	99.293	1.00 17.55	A
40	MOTA	390	N	PHE	68	24 071	-12.839	101 249	1.00 16.84	A .
. •										
	MOTA	391	CA	PHE	68		-11.666		1.00 18.85	A
	MOTA	392	CB	PHE	68	24.119	-10.371	101.340	1.00 17.59	A
	MOTA	393	CG	PHE	68	23.343	-10.206	100.080	1.00 17.32	A
	MOTA	394	CD1		68		-10.823	99.926		
15									1.00 16.89	A
45	MOTA	395	CD2	PHE	68	23.855	-9.447	99.036	1.00 17.68	A
	MOTA	396	CE1	PHE	68	21.387	-10.680	98.752	1.00 15.86	A
	ATOM	397	CE2		68	23.144	-9.296	97.852	1.00 16.89	A
•										
	MOTA	398	CZ	PHE	68	21.906	-9.916	97.708	1.00 17.47	A
	ATOM	399	C	PHE	68	25.641	-11.731	102.745	1.00 19.38	A
50	MOTA	400	0	PHE	68	25.505	-12.703	103.479	1.00 21.74	A
-										
	MOTA	401	N	ASP	69		-10.688		1.00 19.56	A
	MOTA	402	CA	ASP	69	27.105	-10.670	104.344	1.00 20.30	A
	ATOM ·	403	CB	ASP	69	28.177	-9.571	104.313	1.00 20.07	A
	MOTA	404	CG	ASP	69	29.306		103.332	1.00 22.41	A
55										
22	MOTA	405	OD1	ASP	69	29.245	-9.494	102.143	1.00 20.37	Α
	MOTA	406	OD2	ASP ·	69	30.259	-10.582	103.756	1.00 27.46	A
	MOTA	407	C	ASP	69		-10.500		1.00 20.55	A
	ATOM	408	0	ASP	69		-11.073		1.00 20.31	A
	MOTA	409	N	MET	70	25.091	-9.718	105.325	1.00 21.04	Α
60	MOTA	410	CA	MET	70	24.065	-9 469	106.338	1.00 20.59	A
	ATOM									
		411	CB	MET	70	24.464		107.257	1.00 23.87	A
	ATOM	412	CG	MET	70	25.600	-8.650	108.202	1.00 27.55	A
	ATOM	413	SD	MET	70	25.794		109.420	1.00 28.63	A
65	ATOM	414	CE	MET	70	24.665		110.676	1.00 29.22	A
65	MOTA	415	С	MET	70	22.737	, -9.115	105.678	1.00 20.50	A
	ATOM	416	0	MET	70	22.697		104.657	1.00 19.82	A
	ATOM	417	N	VAL	71	21.646		106.258	1.00 18.11	A
	ATOM	418	CA	VAL	71	20.335	-9.289	105.713	1.00 17.48	A
_	ATOM	419	CB	VAL	71	19.701	-10.516	105.021	1.00 17.16	A
70	ATOM	420	CG1		71		-10.915		1.00 14.56	
, ,										A
	ATOM	421	CG2		71		-11.662		1.00 19.68	A
	ATOM	422	С	VAL	71	19.424	-8.791	106.822	1.00 16.09	A
		423	ŏ		71			107.913		
	MOTA	443	U	VAL	/1	19.395	-3.350	101.913	1.00 14.72	A

	MOTA MOTA	424 425	N CA	PHE PHE	72 72	18.714 17.793		106.529 107.460	1.00 16.25 1.00 15.53	A A
	ATOM	426	CB	PHE	72	18.289		107.799	1.00 14.92	A
	ATOM	427	CG	PHE	72	19.575		108.575	1.00 17.03	Ä
5	MOTA	428	CD1	PHE	· 72	19.590	-6.004	109.925	1.00 16.20	A
	MOTA	429		PHE	72	20.782		107.950	1.00 17.34	A
•	MOTA	430		PHE	72	20.785		110.649	1.00 16.42	A
	MOTA	431	CE2	PHE	72	21.979		108.660	1.00 16.87	A
10	MOTA	432	CZ	PHE	72	21.983		110.016	1.00 16.79	A
10	MOTA	433	C	PHE	72 72	16.388		106.874	1.00 15.43	A
	MOTA MOTA	434 435	O N	PHE	73	16.163 15.445		105.834 107.557	1.00 13.98 1.00 18.08	A A
	ATOM	436	CA	GLY	73	14.067		107.104	1.00 17.75	A
	MOTA	437	Ċ	GLY	73	13.343		107.478	1.00 19.38	A
15	ATOM	438	ō	GLY	73	13.918		108.101	1.00 19.14	A
	ATOM	439	N	ALA	74	12.069		107.103	1.00 20.07	A
	MOTA	440	CA	ALA	74	11.228	-5.145	107.363	1.00 20.00	A
	MOTA	441	CB	ALA	74	9.840		106.800	1.00 19.61	A
20	ATOM	442	C	ALA	74	11.124		108.834	1.00 19.69	A
20	MOTA	443	0	ALA	74	10.972		109.123	1.00 21.06	Ā
	MOTA	444	N	SER	75	11.213		109.765	1.00 18.30	A
	MOTA MOTA	445 446	CA CB	SER	75 75	11.103 10.789		111.177 111.991	1.00 18.31 1.00 16.40	Α.
	ATOM	447	OG	SER SER	75 75	11.886		111.971	1.00 15.40	A A
25	ATOM	448	C	SER	75	12.359		111.748	1.00 18.96	Ä
	MOTA	449	ō	SER	75	12.368		112.902	1.00 19.99	Ä
	ATOM	450	N	THR	76	13.407		110.937	1.00 18.45	Ä
	MOTA	451	CA	THR	76	14.667		111.390	1.00 17.88	A
20	MOTA	452	CB	THR	76	15.783	-4.165	110.347	1.00 18.01	A
30	MOTA	453		THR	76	15.861		110.019	1.00 17.20	A
	MOTA	454	CG2	THR	76	17.109		110.902	1.00 17.48	A
	ATOM	455	C	THR	76	14.570		111.687	1.00 17.40	A
	MOTA	456	0	THR	76 77	14.064		110.877	1.00 18.84	A
35	MOTA	457 · 458	N	LYS	77 77	15.061		112.853	1.00 16.09	A
55	MOTA MOTA	459	CA CB	LYS	77	15.032 14.667		113.262 114.751	1.00 17.09 1.00 19.20	A A
	ATOM	460	CG	LYS	77	13.337		115.120	1.00 20.20	Ä
	ATOM	461	CD	LYS	77	12.198		114.302	1.00 24.17	Ä
	MOTA	462	CE	LYS	77	10.882		114.556	1.00 28.56	Ä
40	MOTA	463	NZ	LYS	77	9.741	-0.673	113.832	1.00 29.29	A
	MOTA	464	C	LYS	77	16.383		113.007	1.00 16.81	A
	ATOM	465	0	LYS	77	17.382		112.760	1.00 16.91	A
	MOTA	466	N	GLN	78	16.414		113.067	1.00 14.39	A
45	ATOM ATOM	467 468	CA CB	GLN	78 78	17.657 17.422		112.831	1.00 13.21	A
73	ATOM	469	CG	GLN	78	16.343		112.945 112.017	1.00 10.26 1.00 10.24	A A
	MOTA	470	CD	GLN	78	16.799		110.579	1.00 8.85	Ä
	ATOM	471		GLN	78	17.170		109.922	1.00 10.32	Ä
	ATOM	472	NE2	GLN	78	16.776		110.081	1.00 6.58	A
50	MOTA	473	С	GLN	78	18.750	1.687	113.821	1.00 13.02	A
	ATOM	474	0	GLN	78	19.933		113.474	1.00 11.38	A
	ATOM	475	N	ILE	79	18.352		115.053	1.00 12.89	, A
	ATOM	476	CA	ILE	79	19.313	1.013		1.00 13.42	A
55	ATOM	477	CB	ILE	79 70	18.635		117.479	1.00 13.40	A
55	ATOM ATOM	478 479		ILE	79 79	17.591 19.684		117.508 118.571	1.00 14.83	A
	ATOM	480		ILE	79	20.653		118.775	1.00 13.65 1.00 14.47	A
	ATOM	481	C	ILE	79	19.972		115.771	1.00 12.91	A A
	ATOM	482	ŏ	ILE	79	21.157		116.044	1.00 12.01	Ä
60 -	ATOM	483	N	ASP	80	19:204		115.182	1.00 13.40	A
	MOTA	484	CA	ASP	80	19.719		114.815	1.00 14.93	A
	ATOM	485	СВ	ASP	80	18.581	-3.461	114.303	1.00 17.57	A
	ATOM	486	CG	ASP	80	17.428	-3.593	115.300	1.00 20.41	A
6 5	ATOM	487	OD1		80	17.692		116.504	1.00 22.08	A
65	ATOM	488	OD2		80	16.253		114.879	1.00 21.37	A
	ATOM	489	C	ASP	80	20.777		113.719	1.00 15.46	A
	ATOM ATOM	490	0	ASP	80	21.845		113.769	1.00 15.07	A
	MOTA MOTA	491 492	N CA	VAL VAL	81 81	20.467 21.380		112.730 111.625	1.00 15.97 1.00 16.25	A
70	MOTA	493	CB	VAL	81	20.747		110.555	1.00 16.25	A A
	ATOM	494	CG1		81	21.787		109.526	1.00 14.56	A
	ATOM	495	CG2		81	19.568		109.857	1.00 14.48	Ä
	MOTA	496	C	VAL	81	22.667		112.142	1.00 18.57	A

	ATOM	497	0	VAL	81	23.758	-1.079 1	11.733	1.00 20.96	Α
	ATOM	498	N	TYR	82	22.549	0.289 1		1.00 19.05	A
	ATOM	499	CA	TYR	82	23.732	0.946 1		1.00 20.41	A
	ATOM	500	CB	TYR	82	23.339			1.00 23.17	A
5	ATOM	501	CG	TYR	82	24.532	2.903 1		1.00 24.73	A
_	ATOM	502		TYR	82	25.137	2.556 1		1.00 24.58	Ä
	ATOM	503		TYR	82	26.284	3.200 1		1.00 25.15	Ä
	ATOM	504		TYR	82	25.107	3.928 1		1.00 25.38	A
	ATOM	505	CE2		82	26.258			1.00 25.61	A
10	ATOM	506	CZ	TYR	82	26.842	4.204 1		1.00 25.89	À
	MOTA	507	ОН	TYR	82	28.000	4.818 1		1.00 26.74	Ä
	MOTA	508	C	TYR	82	24.633	-0.002 1		1.00 20.74	A
	ATOM ·		ŏ	TYR	82	25.835	-0.104 1		1.00 22.10	
	ATOM	510	N	ARG	83	24.059				A
15	ATOM	511	CA	ARG		24.834	-0.694 11 -1.615 11		1.00 21.11	A
13	ATOM	512	CB	ARG	83 83	23.928				A
	ATOM	513	·CG				-2.263 11		1.00 18.85	A
	ATOM	514	CD	ARG	83	23.521	-1.315 11		1.00 21.14	A
			NE	ARG	83	22.272	-1.804 11		1.00 21.88	A
20	ATOM	515		ARG	83	22.478	-3.061 11		1.00 22.27	A
20	MOTA	516	CZ	ARG	83	23.184	-3.175 12		1.00 23.18	A
	MOTA	517		ARG	83	.23.757	-2.104 13		1.00 23.11	A
	ATOM ·	518	NH2		83	23.308	-4.356 13		1.00 23.57	A
	MOTA	519	C	ARG	83	25.553	-2.694 11		1.00 19.49	A
25	ATOM	520	0	ARG	83	26.702	-3.022 13		1.00 17.49	A
23	ATOM	521	N	SER	84	24.885	-3.225 13		1.00 19.74	· A
	ATOM	522	CA	SER	84	25.462	-4.283 13		1.00 19.67	A
	MOTA	523	CB OG	SER	84	24.359	-5.135 11		1.00 21.49	A
	ATOM ATOM	524 525	C	SER	84	23.716	-5.931 11		1.00 28.64	A
30	ATOM	526		SER	84	26.419	-3.859 11 -4.436 11		1.00 18.56	A
50	ATOM		0		84	27.487 26.058			1.00 19.77	A
		527 528	N	VAL VAL	85		-2.866 13		1.00 18.63	A
	ATOM		CA		85 05	26.949 26.161	-2.470 13		1.00 19.52	A
	MOTA MOTA	529 530	CB	VAL VAL	85		-2.241 10 -3.377 10		1.00 19.26	A
35	ATOM				85 85	25.165			1.00 20.45	A
55	ATOM	531 532		VAL VAL	85	25.448	-0.925 10		1.00 22.19	A
	ATOM	533	C	VAL	85 85	27.828	-1.252 11		1.00 19.41	A
	MOTA		0		85 86	29.034	-1.289 11		1.00 19.81	A
		534	N	VAL	86 86	27.236	-0.189 11		1.00 19.42	A
40	MOTA	535	CA CB	VAL	86 06	27.959	1.053 11		1.00 19.60	A
70	MOTA	536	CB	VAL	86	26.971	2.226 11		1.00 18.59	A
	MOTA	537		VAL	86 96	27.724	3.545 11		1.00 19.00	A
	MOTA	538		VAL	86	25.899	2.208 11		1.00 18.56	A
	MOTA	539	C	VAL	86	28.950	1.067 11		1.00 20.31	A
45	MOTA	540 541	O N	VAL	86	30.060	1.584 11		1.00 19.36	A
73	ATOM ATOM	542	CA	CYS	87 87	28.559 29.438	0.519 11		1.00 21.30	A
	MOTA	543	CB	CYS	87	28.777	0.535 13		1.00 23.03	A
	ATOM	544	SG	CYS	87	29.481	0.238 11		1.00 26.09	A
	MOTA	545	C	CYS	87	30.824	-0.056 13			A
50	MOTA	546	Ö	CYS	87	31.835	0.546 13		1.00 21.77 1.00 21.30	A
50	ATOM	547	N	PRO	88	30.894	-1.241 11		1.00 20.49	A
	MOTA	548	CD	PRO	88	29.856	-2.240 13		1.00 20.43	A A
	ATOM	549	CA	PRO	88	32.231	-1.783 11		1.00 20.97	Ä
	ATOM	550	СВ	PRO	88	31.948	-3.215 11		1.00 18.41	Ä
55	ATOM	551	CG	PRO	88	30.571	-3.133 11		1.00 20.02	Ä
<i></i>	MOTA	552	C	PRO	. 88	33.052	-0.988 11		1.00 20.02	A
	ATOM	553	ŏ	PRO	88	34.280	-0.937 11		1.00 22.69	
	ATOM	554	N	ILE	89	32.380	-0.373 13		1.00 22.03	A
	MOTA	555	CA	ILE	89	33.068	0.417 13		1.00 20.39	A A
60	MOTA	556	CB	ILE	89	32.130	0.723 10		1.00 20.42	
OO	MOTA	557	CG2		89	32.791	1.710 10		1.00 20.42	A
	ATOM	558	CG1		89	31.786	-0.584 10		1.00 20.17	A
	ATOM	559	CD1		89	30.749				A
	ATOM	560	CDI	ILE	89	33.577	-0.429 10 1.724 11		1.00 21.44 1.00 21.10	. A
65	ATOM	561	0	ILE	89	34.640	2.214 11			· A
55	ATOM	562							1.00 22.45	A
	ATOM	563	N Cz	LEU	90 90	32.818	2.287 11 3.522 11		1.00 20.96	A
	ATOM	564	CA	LEU	90	33.229			1.00 20.72	A
	ATOM	565	CB CG	LEU LEU	90	32.086 32.407	4.094 11 5.390 11		1.00 18.19	A
70	ATOM	566							1.00 19.36	A
, ,	ATOM	567	CD1		90 90	32.779	6.495 11		1.00 17.91	A
	ATOM	568	CD2		90	31.203	5.799 13 3.248 13		1.00 19.74	A
	MOTA	569	С 0	LEU	90	34.443 35.346			1.00 21.43	A
	A I OM	707	V	LEU	90	33.340	4.081 11	4.009	1.00 22.10	A

•	АТОМ	570	N	ASP	91	34.471	2.084	114.632	1.00	21.61	A
	MOTA	571	CA	ASP	91	35.611		115.476		22.75	A
	ATOM	572	CB	ASP	91	35.404		116.172		22.67	A
5	MOTA	573	CG	ASP	91	34.535		117.410		25.39	A
J	MOTA MOTA	574 575	OD2	ASP ASP	91 91	34.386 34.006		117.947 117.859		24.95 27.30	A A
	ATOM	576	C	ASP	91	36.877		114.618		22.42	À
	ATOM	577	õ	ASP	91	37.956		115.077		20.39	A
	ATOM	578	N	GLU	92	36.749		113.378		20.58	A
10	ATOM	579	CA	GLU	92	37.907		112.499		22.88	A
	MOTA	580	·CB	GLU	92	37.599		111.238		24.90	A
	MOTA	581	CG	GLU	92	38.131		111.282	1.00	31.75	A
	MOTA	582	CD	GLU	92	38.517		109.902		35.40	A
15	MOTA	583		GLU	92	39.330		109, 203		36.87	A
13	MOTA MOTA	584		GLU	92 92	38.017		109.519		37.95	A
•	ATOM	585 586	C	GLU	92	38.358 39.554		112.100 111.964		22.24	A A
	MOTA	587	N	VAL	93	37.398		111.909		20.21	A
	ATOM	588	CA	VAL	93	37.712		111.532		18.97	Ä
20	MOTA	589	CB	VAL	93	36.422		111.228		17.93	A
	MOTA	590		VAL	93	36.755		111.094	1.00	14.46	A
	MOTA	591		VAL	93	35.781		109.937		16.29	Α,
	ATOM	592	C	VAL	93	38.489		112.657		19.09	A
25	MOTA MOTA	593	0	VAL	93 94	39.477		112.414		18.02	Α
LJ	MOTA	594 595	N CA	ILE	94	38.044 38.690		115.056		19.70 21.90	A A
	ATOM	596	CB	ILE	94	37.815		116.317		22.69	Ä
	ATOM	597		ILE	94	38.519		117.571		22.60	A
	MOTA	598		ILE	94	36.472		116.124		22.49	A
30	MOTA	599	CD1	ILE	94	35.480		117.266	1.00	22.50	A
	MOTA	600	C	ILE	94	40.116		115.265		24.26	A
	ATOM	601	0	ILE	94	40.924		115.945		24.34	A
	ATOM ATOM	602 603	N CA	MET	95 95	40.428 41.767		114.672		25.73 27.17	A
35	MOTA	. 604	CB	MET	95 95	41.732		114.777 114.532		29.33	A A
-	MOTA	605	CG	MET	95	41.102		115.643		35.68	Ä
	MOTA	606	SD	MET	95	41.281		115.337		44.01	A
	MOTA	607	CE	MET	95	39.718		114.541		39.10	A
40	MOTA	608	С	MET	95	42.722	4.183	113.761	1.00	27.37	A
40	MOTA	609	0	MET	95	43.907		113.711		26.10	A
	MOTA	610	N	GLY	96	42.197		112.939		26.75	A
	MOTA MOTA	611 612	CA	GLY	96 96	43.020 42.861		111.941 110.529		26.52	A
	ATOM	613	ò	GLY	96	43.752		109.690	1.00	25.69	A A
45	MOTA	614	N	TYR	97	41.720	4.597		1.00		Ä
	ATOM	615	CA	TYR	97	41.439		108.949		24.96	A
	MOTA	616	CB	TYR	97	40.932	2.592	109.113	1.00	29.74	A
	MOTA	617	CG	TYR	97	42.007		109.444	1.00		A
50	MOTA	618		TYR	97	42.993		108.514		36.66	A
50	ATOM ATOM	619 620		TYR TYR	97 97	43.970 42.025		108.798		39.73 35.77	A A
	ATOM	621	CE2	TYR	97	42.998		110.979		38.01	À
	MOTA	622	cz	TYR	97	43.969		110.033		40.42	Ä
	MOTA	623	OH	TYR	97	44.956		110.325	1.00		A
55	MOTA	624	С	TYR	97	40.407		108.163	1.00	22.65	A
	MOTA	625	0	TYR	97	39.749		108.711	1.00		A
	MOTA	626	N	ASN	98	40.290		106.872		19.89	A
	MOTA MOTA	627 628	CA	ASN ASN	98 98	39.312		106.021		18.57	Α.
60 ·	ATOM	629	CB CG	ASN	98	39.941 40.867		104.702		19.70 21.50	A A
•	MOTA	630		ASN	98	40.543		105.574	1.00		Ä
	MOTA	631		ASN	98	42.020		104.222		20.02	Ä
	MOTA	632	С	ASN	98	38.195		105.713	1.00		A
65	MOTA	633	0	ASN	98	38.459	3.087	105.346	1.00	16.93	A
65	MOTA	634	N	CYS	99	36.949		105.865	1.00		A
	ATOM	635	CA	CYS	99	35.825		105.575		17.76	A
	MOTA	636	CB	CYS	99	35.244		106.867		18.42	A
	ATOM ATOM	637 638	SG C	CYS	99 99	36.378		107.771	1.00		A
70	ATOM	639	0	CYS	99	34.727 34.508		104.790 104.920	1.00 1.00		A A
. •	ATOM	640	N	THR	100	34.044		103.968	1.00		À
	MOTA	641	CA.	THR	100	32.968		103.130	1.00		Ä
	MOTA	642	CB	THR	100	33.417		101.657	1.00		A

	ATOM	643	OG1	THR	100	34.485	5.223	101.539	1.00 14.13	A
	ATOM	644	CG2	THR	100	32.262	4.717	100.773	1.00 12.44	A
	MOTA	645	C	THR	100	31.759	3.260	103.200	1.00 14.15	A
_	ATOM	646	0	THR	100	31.907		103.263	1.00 13.80	Ä
5	ATOM	647	N	ILE	101	30.568		103.199	1.00 12.37	A
	ATOM	648	CA	ILE	101	29.329		103.202	1.00 11.07	A
	ATOM	649	СВ	ILE	101	28.608		104.551	1.00 10.99	A
	ATOM	650		ILE	101	27.404		104.527	1.00 11.07	A
	ATOM	651		ILE	101	29.551		105.682	1.00 11.36	
10	ATOM	652		ILE	101	28.880				A
	MOTA	653	CDI	ILE	101	28.394		107.071	1.00 11.31	A
		654						102.123	1.00 10.34	· A
	MOTA		0	ILE	101	28.077		102.133	1.00 8.62	A
	MOTA	655	N	PHE	102	27.980		101.192	1.00 8.88	A
15	ATOM	656	CA	PHE	102	27.089		100.113	1.00 8.18	A
15	ATOM	657	CB	PHE	102	27.521	2.554	98.798	1.00 8.39	A
	MOTA	658	CG	PHE	102	28.786	3.107	98.212	1.00 8.44	A
	MOTA	659		PHE	102	28.746	4.237	97.400	1.00 8.21	A
	MOTA	660		PHE	102	30.004	2.449	98.402	1.00 7.42	A
20	ATOM	661	CE1	PHE	102	29.901	4.712	96.770	1.00 10.64	A
20	MOTA	662	CE2	PHE	102	31.167	2.910	97.780	1.00 9.88	A
	ATOM	663	ÇZ	PHE	102	31.119	4.044	96.957	1.00 10.26	A
	ATOM ·	664	С	PHE	102	25.686	2.695	100.418	1.00 9.34	A
	ATOM	665	0	PHE	102	25.514		101.084	1.00 9.83	A
	ATOM	666	N	ALA	103	24.686	3.420	99.937	1.00 8.83	A
25	ATOM	667	CA	ALA	103	23.301		100.088	1.00 6.41	A
	ATOM	668	CB	ALA	103	22.503		100.836	1.00 6.59	. Ä
	ATOM	669	C	ALA	103	22.887	2.920	98.619	1.00 5.06	A
	MOTA	670	ō	ALA	103	22.988	3.898	97.890	1.00 3.08	Ä
	MOTA	671	N	TYR	104	22.476	1.735	98.184	1.00 4.26	
30	ATOM	672	CA	TYR	104	22.110	1.498	96.791		A
	ATOM	673	СВ	TYR	104	23.142	0.552	96.137	1.00 4.91	A
	ATOM	674	CG	TYR	104	22.911			1.00 3.89	A
	MOTA	675		TYR	104	21.933	0.238	94.666	1.00 4.19	A
	ATOM	676					-0.675	94.260	1.00 6.04	A
35	MOTA			TYR	104	21.722	-0.946	92.898	1.00 7.93	A
55		677	CD2	TYR	104	23.667	0.868	93.679	1.00 5.77	A
	MOTA	678		TYR	104	23.466	0.608	92.326	1.00 5.74	A
	MOTA	679	CZ	TYR	104	22.500	-0.295	91.944	1.00 6.93	A
	MOTA	680	ОН	TYR	104	22.326	-0.551	90.604	1.00 8.61	A
40	ATOM	681	C	TYR	104	20.718	0.893	96.678	1.00 5.23	A _.
40	ATOM	682	0	TYR	104	20.346	0.007	97.445	1.00 7.02	A
	ATOM	683	N	GLY	105	19.955	1.368	95.704	1.00 3.82	A
	ATOM	684	CA	GLY	105	18.620	0.857	95.521	1.00 5.02	A
	ATOM	685	С	GLY	105	17.705	1.803	94.773	1.00 5.87	A
	ATOM	686	0	GLY	105	17.981	2.992	94.590	1.00 6.06	À
45	ATOM	687	N	GLN	106	16.598	1.244	94.326	1.00 4.13	A
	ATOM	688	CA	GLN	106	15.601	1.986	93.591	1.00 6.44	A
	ATOM	689	CB	GLN	106	14.513	0.998	93.158	1.00 6.41	A
	ATOM	690	CG	GLN	106	13.175	1.585	92.817	1.00 11.96	A
	MOTA	691	CD	GLN	106	12.136	0.511	92.499	1.00 14.57	Ä
50	MOTA	692	OE1		106	12.060	-0.539	93.172	1.00 12.16	A
	ATOM	693	NE2		106	11.318	0.774	91.483	1.00 10.80	A
	ATOM	694	С	GLN	106	15.047	3.091	94.488	1.00 7.89	
		695	ŏ	GLN	106	15.083	2.992	95.725	1.00 8.30	A
	ATOM	696	N	THR	107	14.558	4.157	93.869		A
55	ATOM	697	CA	THR	107	13.981			1.00 8.49	A
-	ATOM	698	CB	THR	107		5.259	94.620	1.00 8.83	A
	ATOM					13.532	6.371	93.668	1.00 10.17	A
		699	0G1		107	14.681	6.936			A
	ATOM	700	CG2		107	12.783	7.464	94.431	1.00 9.05	A
60	MOTA	701	C	THR	107	12.763	4.751	95.392	1.00 11.60	` A
UU	ATOM	702	0	THR	107	11.936	4.017	94.838	1.00 13.74	A
	MOTA	703	N	GLY	108	12.661	5.121	96.668	1.00 11.74	A
	MOTA	704	CA	GLY	108	11.527	4.703	97.476	1.00 9.99	A
	MOTA	705	C	GLY	108	11.738	3.461	98.330	1.00 11.25	A
65	MOTA	706	0	GLY	108	10.812	3.004	99.018	1.00 12.52	A
65	MOTA	707	N	THR	109	12.947	2.915	98.313	1.00 9.04	A
	ATOM	708	CA	THR	109	13.216	1.716	99.090	1.00 8.13	A
	MOTA	709	CB	THR	109	14.053	0.703	98.291	1.00 8.11	A
	MOTA	710	OG1		109	15.274	1.321	97.857	1.00 5.32	Ä
	MOTA	711	CG2		109	13.269	0.220	97.079	1.00 2.18	Â
70	MOTA	712		THR	109	13.914		100.405	1.00 8.77	Ä
	MOTA	713		THR	109	14.029		101.236	1.00 9.56	A
	ATOM	714		GLY	110	14.411		100.599	1.00 6.93	
	ATOM	715		GLY	110	15.037		100.333	1.00 6.93	A
						43.037	3.311	-01.0/0	1.00 /.00	A

•	ATOM	716	С	GLY	110		16.491	3.959	101.985	1.00	8.39	A
	MOTA	717	0	GLY	110		17.052	3.953	103.089	1.00	6.64	A
	MOTA	718	N	LY5	111		17.106		100.869	1.00	8.77	A
5	MOTA	719	CA	LYS	111		18.493	-	100.888	1.00	8.41	A
3	MOTA	720	CB	LYS	111		18.938	5.257	99.495	1.00	9.46	A
	ATOM	721	CG	LYS	111		19.086	4.134	98.462	1.00	8.41	Ą
	ATOM ATOM	722 723	CD	LYS LYS	111 111		19.650 18.772	4.651 5.741	97.133 96.526	1.00	7.10 8.55	A A
	MOTA	724	NZ	LYS	111		17.364	5.298	96.325	1.00	7.14	A
10	ATOM	725	C	LYS	111		18.643		101.862	1.00	8.34	A
	ATOM	726	٠ō	LYS	111		19.448		102.789	1.00	9.08	A
	ATOM	727	N	THR	112		17.851		101.651	1.00	8.83	À
	ATOM-	728	CA	THR	112		17.896		102.502	1.00	7.73	A
	MOTA	729	CB	THR	112		17.027	9.342	101.903	1.00	8.07	A
15	MOTA	730		THR	112		17.347		100.502	1.00	8.01	A
	MOTA	731		THR	112		17.287		102.650	1.00	4.02	A
	MOTA	732	C	THR	112		17.454		103.945	1.00	8.81	A
	MOTA MOTA	733 734	O N	THR	112 113		17.997 16.476		104.894	1.00	8.08	A A
20	MOTA	735	CA	PHE	113		16.008		105.448		11.03	A
	ATOM	736	СВ	PHE	113		14.806		105.361		10.34	Ä
	MOTA	737	CG	PHE	113		14.208		106.699		10.76	A.
	MOTA	738	CD1	PHE	113		13.247	6.214	107.276	1.00	9.64	A
25	MOTA	739		PHE	113		14.623		107.393	1.00	9.33	· A
25	MOTA	740		PHE	113		12.703		108.523		10.99	A
	MOTA	741		PHE	113		14.084		108.646		11.97	A
	MOTA MOTA	742	CZ	PHE	113		13.120		109.212	1.00	9.40	A
	ATOM	743 744	0	PHE	113 113	•	17.120 17.254		106.205		11.21	A
30	ATOM	745	N	THR	114		17.908		105.483		10.89	A A
-	ATOM	746	CA	THR	114		18.992		106.101	1.00	9.91	À
	ATOM	747	СВ	THR	114		19.458		105.173		12.09	A
	MOTA	748	.0G1	THR	114		18.375		105.001		10.83	A
25.	MOTA	749		THR	114		20.677	2.537	105.763	1.00	9.73	A
35		750	C	THR	114		20.167		106.438		10.11	A
•	ATOM	751	0	THR	114		20.650		107.569		10.60	A
	MOTA	752	N	MET	115		20.606		105.466		11.39	A
	MOTA MOTA	753 754	CA CB	MET	115 115		21.745 22.286		105.666		11.76 14.08	A
40	ATOM	755	CG	MET	115		22.774		103.406		21.28	A A
. •	ATOM	756	SD	MET	115		24.093		104.142		28.02	Ä
	ATOM	757	CE	MET	115		25.184		104 670		16.59	Ä
•	MOTA	758	Ċ	MET	115		21.489	8.240	106.547	1.00	11.39	A
45	ATOM	759	0	MET	115		22.347		107.349		11.70	A
45	ATOM	760	N	GLU	116		20.322		106.410		10.32	A
	MOTA	761	CA	GLU	116		20.023		107.197	1.00	9.04	λ
	ATOM ATOM	762 763	CB CG	GLU	116 116		19.498 20.215		106.299 104.970		11.83 15.21	A A
	ATOM	764	CD	GLU	116		19.911		104.319		17.70	Ä
50	MOTA	765		GLU	116		18.751		104.405		20.63	A
	MOTA	766	OE2	GLU	116		20.830		103.715		19.36	A
	MOTA	767	C	GLU	116 .		19.021		108.319	1.00	8.57	A
	ATOM	768	0	GLU	116		19.225		109.430	1.00	6.66	A
55	ATOM	769	N	GLY	117		17.937		108.024		10.69	A
55	ATOM ATOM	770 771	CA	GLY GLY	117 117		16.894 15.906		109.011		12.05	A
	ATOM	772	ŏ	GLY	117		16.009		108.921		14.49 15.09	A
	ATOM	773	N	GLU	118		14.954		109.844		15.27	A A
	ATOM	774	CA	GLU	118		13.955		109.827		17.05	A
60 ·	ATOM	775	CB	GLU	118		12.680		109.132		18.95	A
	ATOM	776	CG	GLU	118		12.881	10.219	107.732		24.85	A
	MOTA	777	CD	GLU	118		11.659		107.228		28.50	A
	MOTA	778		GLU	118		11.639		106.047		29.02	A
65	MOTA	779		GLU	118		10.715		108.025		31.54	A
05	ATOM ATOM	780 781	C	GLU	118		13.601		111.246		15.85	A
	ATOM	781 782	O N	GLU ARG	118 119		14.159		112.206 111.381		17.29	A
	ATOM	783	CA	ARG	119		12.660 12.238		111.381		14.03 12.36	A A
	ATOM	784	CB	ARG	119		12.058		112.765	1.00	9.51	A
70	MOTA	785	CG	ARG	119		13.311		112.459	1.00	9.85	Ä
	MOTA	786	CD	ARG	119		14.517		113.223	1.00	9.11	Ä
	MOTA	787	NE.	ARG	119		14.226	14.503	114.632	1.00	11.37	A
	MOTA	788	CZ	ARG	119		14.274	15.409	115.601	1.00	9.83	A

	ATOM	789	NH1	ARG	119	14.607	16.663	115.326	1.00 8.80	A
	MOTA	790		ARG	119	14.003		116.851	1.00 8.38	A
	MOTA	791	C	ARG	119	10.909		113.012	1.00 13.30	A
_	MOTA	792	0	ARG	119	10.055		112.140	1.00 12.33	λ
5	MOTA	793	N	SER	120	10.746		114.244	1.00 14.08	A
	ATOM	794	CA	SER	120	9.478		114.630	1.00 14.63	· A
	ATOM	795	CB	SER	120	9.563	10.651	116.037	1.00 13.18	A
	MOTA	796	OG	SER	120	10.380	9.500	116.043	1.00 13.75	A
4.6	MOTA	797	С	SER	120	8.542	12.434	114.610	1.00 14.70	A
10	MOTA	798	0	SER	120	8.966	13.556	114.877	1.00 14.22	A
	MOTA	799	N	PRO	121	7.263	12.222	114.295	1.00 15.80	Α
	MOTA	800	CD	PRO	121	6.629	10.969	113.860	1.00 15.88	A
	MOTA	801	CA	PRO	121	6.312	13.340	114.253	1.00 16:98	A
1.5	MOTA	802	CB	PRO	121	5.037		113.703	1.00 17.68	A
15	MOTA	803	CG	PRO	121	5.528	11.476	112.967	1.00 1B.94	A
	ATOM	804	С	PRO	121	6.036		115.589	1.00 17.31	A
	ATOM		. 0	PRO	121	6.316		116.662	1.00 17.01	A
	MOTA	806	N	ASN	122	5.493		115.498	1.00 18.27	A
20	ATOM	807	CA	ASN	122	5.079		116.659	1.00 19.75	A
20	ATOM	808	CB	ASN	122	3.899		117.323	1.00 22.14	A
	ATOM	809	CG	ASN	122	2.806		117.782	1.00 25.67	λ
	ATOM ·	810		ASN	122	2.331		117.020	1.00 28.24	A
	ATOM	811		ASN	122	2.386		119.029	1.00 29.36	À
25	ATOM ATOM	812 813	0	ASN ASN	122 122	6.137 5.810		117.714	1.00 20.30	A
	ATOM	814	N	GLU	123	7.398		118.889	1.00 19.52	A
	ATOM	815		GLU	123	8.460		117.312 118.267	1.00 20.21	. A
	ATOM	816	CB	GLU	123	8.341		118.781	1.00 21.19	A A
	ATOM	817	CG	GLU	123	8.519		117.731	1.00 20.11	A
30	ATOM	818	CD	GLU	123	8.575		118.319	1.00 21.92	Ä
	ATOM	819		GLU	123	7.688		119.133	1.00 18.15	Ä
		820		GLU	123	9.507		117.951	1.00 21.94	A
	ATOM	821	c	GLU	123.	8.446		119.468	1.00 21.37	Ä
	MOTA	822	0	GLU	123	8.632		120.602	1.00 19.07	A
35	MOTA	823	N	GLU	124	8.226	14.518	119.233	1.00 22.79	A ·
	ATOM	824	CA	GLU	124	8.210		120.339	1.00 22.88	A
	MOTA	825	CB	GLU	124	7.685	12.215	119.887	1.00 25.26	A
	MOTA	826	CG	GLU	124	7.600	11.205	121.033	1.00 30.44	A
40	MOTA	827	CD	GLU	124	6.924	9.899	120.636	1.00 34.84	Α
40	MOTA	828		GLU	124	6.827	9.003	121.508	1.00 33.81	À
	MOTA	829		GLU	124	6.494		119.464	1.00 37.51	A
	MOTA	830	C.	GLU	124	9.592		120.964	1.00 22.45	A
	MOTA	831	0	GLU	124	9.715		122.180	1.00 23.30	A
45	MOTA	832	N	TYR	125	10.635		120.142	1.00 20.18	Ά
77	MOTA	833 834	CA	TYR	125	11.988		120.657	1.00 19.15	λ
	ATOM ATOM	835	CB CG	TYR TYR	125 125	12.602		120.150	1.00 17.84	A
	ATOM	836	CD1		125	11.805 10.791		120.391 119.513	1.00 17.89	A
	ATOM	837	CE1		125	10.791		119.513	1.00 18.58 1.00 18.72	A
50	ATOM	838	CD2		125	12.090		121.477	1.00 18.72	A A
	MOTA	839		TYR	125	11.395		121.686	1.00 17.82	A
	ATOM	840	cz	TYR	125	10.398		120.804	1.00 19.43	Ä
	ATOM	841	OH	TYR	125	9.724		121.017	1.00 23.55	A
	MOTA	842	C	TYR	125	12.941		120.260	1.00 18.68	A
55	MOTA	843	0	TYR	125	12.678		119.338	1.00 20.06	A
	MOTA	844	N	THR	126	14.061	14.445	120.971	1.00 18.30	A
	ATOM	845	CA	THR	126	15.106	15.402	120.651		A
	MOTA	846	CB	THR	126	16.063	15.618	121.839	1.00 18.63	A
	ATOM	847	0G1	THR	126	16.592	14.356	122.254	1.00 20.05	A
60	MOTA	848	CG2	THR	126	15.339	16.258	123.014	1.00 18.83	A
	MOTA	849	С	THR	126	15.838	14.653	119.537	1.00 17.89	A
	MOTA	850	0	THR	126	15.606		119.355	1.00 16.79	A
	ATOM	851	N	TRP	127	16.708		118.789	1.00 16.50	A
65	ATOM	852	CA	TRP	127	17.401		117.711	1.00 16.42	A
65	MOTA	853		TRP	127	18.198		116.868	1.00 14.53	A
	MOTA	854	CG	TRP	127	19.443		117.506	1.00 12.21	A
	MOTA	855	CD2		127	20.746		117.381	1.00 12.40	A
	MOTA	856	CE2		127	21.634		118.138	1.00 12.89	A
70	MOTA	857	CE3		127	21.250		116.703	1.00 10.82	A
,,,	MOTA	858 850	CD1		127	19.580		118.314	1.00 12.48	A
	MOTA MOTA	859 860	NE1		127	20.899		118.698	1.00 14.38	A
	ATOM	860 861	CZ2		127 127	22.997		118.233	1.00 12.67	A
	A I OF	001	C23	IRP	121	22.607	14.149	116.800	1.00 8.68	A

	ATOM	862	CH2	TRP	127		23.463	14.959	117.558	1.00 10.75	Α
	ATOM	863	C	TRP	127	•					
							18.318		118.191	1.00 18.04	A
	MOTA	864	0	TRP	127		18.496	12.507	117.491	1.00 17.73	Α
	ATOM	865	N	GLU	128		18.874	13 630	119.390	1.00 20.55	A
5											
9	ATOM	866	CA	GLU	128		19.773		119.954	1.00 22.98	A
	MOTA	867	CB	GLU	128		20.449	13.167	121.216	1.00 24.66	A
	MOTA	868	CG	GLU	128		21.328		121.028	1.00 30.86	A
	MOTA	869	CD	GLU	128		21.812	14.929	122.359	1.00 34.39	A
	MOTA	870	OE1	GLU	128		22.271	14.126	123.204	1.00 36.58	A
10											
10	ATOM	871	OE2		128		21.734		122.562	1.00 36.22	A
	MOTA	872	·C	GLU	128		19.092	11.322	120.336	1.00 21.59	A
	MOTA	873	0	GLU	128		19.744	10 201	120.456	1.00 20.67	A
	MOTA	874	N	GLU	129		17.784		120.539	1.00 22.17	A
	MOTA	875	CA	GLU	129		17.073	10.167	120.974	1.00 22.68	A
15	ATOM	876	CB	GLU	129		16.487		122.364	1.00 23.27	
1.5											A
	MOTA	877	CG	GLU	129		17.550	10.770	123.392	1.00 28.13	A
	ATOM	878	CD	GLU	129		16.965	11.157	124.737	1.00 32.95	A
	ATOM	879									
				GLU	129		17.752		125.702	1.00 33.26	A
	MOTA	880	OE2	GLU	129		15.724	11.301	124.827	1.00 31.63	Α
20 T	MOTA	881	С	GLU	129		15.983	9 679	120.035	1.00 20.72	. А
	ATOM	882	ŏ								
				GLU	129		15.273		120.343	1.00 23.09	A
	MOTA	883	N	ASP	130		15.862	10.322	118.885	1.00 18.40	A
	MOTA	884	CA	ASP	130		14.846	9.945	117.918	1.00 16.36	A
25	ATOM	.885	СВ	ASP	130		14.770		116.828	1.00 15.71	·A
25	MOTA	886	CG	ASP	130		13.495	10.947	116.031	1.00 15.49	A
	MOTA	887	OD1:	ASP	130		13.044	12 002	115.545	1.00 17.27	A
	MOTA	888	QDZ	ASP	130		12.950		115.874	1.00 15.06	A
	ATOM	889	С	ASP	130		15.168	8.573	117.326	1.00 15.41	A
	MOTA	890	0	ASP	130		16.196		116.680	1.00 15.65	Ä
30											
30	MOTA	891	N	PRO	131		14.287	7.597	117.548	1.00 14.81	A
	ATOM	892	CD	PRO	131		12.980	7.675	118.222	1.00 14.52	A
	ATOM	893	CA	PRO	131		14.523		117.018		
										1.00 15.02	A
	MOTA	894	CB	PRO	131		13.348	5.457	117.579	1.00 15.21	A
	ATOM	895	CG	PRO	131		12.267	6:478	117.656	1.00 16.02	A
35 ·		896	Č	PRO	131				115.492		
55							14.607			1.00 15.04	A
	ATOM	897	0	PRO	131		15.103	5.196	114.943	1.00 12.71	A
	ATOM	898	N	LEU	132		14.125	7.224	114.814	1.00 14.88	A
	ATOM	899	CA	LEU	132		14.161		113.354	1.00 14.03	A
	ATOM	900	CB	LEU	132		12.947	8.007	112.796	1.00 12.82	A
40	ATOM	901	CG	LEU	132		11.562		113.129	1.00 14.44	A
. •											
	MOTA	902	CD1		132		10.506	8.271	112.397	1.00 8.97	A
	MOTA	903	CD2	LEU	132		11.470	5.950	112.724	1.00 8.90	A
	MOTA	904	С	LEU	132		15.446		112.786	1.00 12.21	A
40	MOTA	905	0	LEU	132		15.626	7.916	111.573	1.00 11.16	A
45	ATOM	906	N	ALA	133		16.337	8.321	113.655	1.00 11.83	A
	ATOM	907	CA	ALA	133		17.604		113.186		
										1.00 11.94	A
	ATOM	908	CB	ALA	133		18.447	9.345	114.377	1.00 7.70	A
	ATOM	909	С	ALA	133		18.367	7.825	112.373	1.00 12.53	A
	ATOM	910	ō	ALA	133		18.308				
50								6.637		1.00 12.95	A
<i>5</i> 0	MOTA .	911	N	GLY	134		19.074	8.256	111.330	1.00 13.23	A
	MOTA	912	CA	GLY	134		19.832	7.328	110.506	1.00 13.31	A
	MOTA	913	С	GLY	134		21.314		110.858	1.00 14.51	
											A
	MOTA	914	0	GLY	134		21.727	7.771	111.910	1.00 12.96	A
	MOTA	915	N	ILE	135		22.111	6.685	109.962	1.00 13.27	A
55	ATOM	916	CA	ILE	135		23.547		110.158	1.00 10.64	
-											A
	MOTA	917	CB	ILE	135		24.211	5.825	108.945	1.00 12.21	A
	MOTA	918	CG2	ILE	135		25.728	5.725	109.166	1.00 9.26	A
	MOTA	919	CG1		135		23.606		108.749		
											A
/ 0	ATOM	920	CD1	ILE	135		24.194	3.659	107.563	1.00 7.34	A
60 ·	ATOM	921	С	ILE	135		24.319	7.817	110.429	1.00 11.04	A
	ATOM	922	ŏ	ILE	135				111.370		
							25.101	-		1.00 12.98	A
	MOTA	923	N	ILE	136		24.117	8.843	109.606	1.00 10.10	A
	MOTA	924	CA	ILE	136		24.822		109.783	1.00 10.16	A
45	MOTA	925	CB	ILE	136		24.393		108.709	1.00 9.76	A
65	MOTA	926	CG2	ILE	136		25.052	12.489	108.966	1.00 7.05	A
	ATOM	927	CG1		136		24.783		107.327	1.00 8.04	
											A
	MOTA	928	CD1		136		24.420		106.177	1.00 8.70	A
	ATOM	929	C	ILE	136		24.680	10.734	111.180	1.00 10.98	A
	ATOM .	930	õ	ILE	136		25.673		111.848	1.00 11.07	
70											A
<i>,</i> σ	MOTA	931	N	PRO	137		23.449	11.015	111.637	1.00 12.76	, A
	ATOM	932	CD	PRO	137		22.118	10.891	111.018	1.00 12.91	. A
	ATOM	933	CA.		137				112.974		
							23.344			1.00 13.27	A
	MOTA	934	CB	PRO -	137		21.863	11.966	113.079	1.00 12.28	A

	ATOM	935	CG	PRO	137	21.210	10.920	112.226	1.00 12.44	A
	ATOM	936	Ċ	PRO	137	23.814		114.117	1.00 13.75	A
	MOTA	937	0	PRO	137	24.349		115.118	1.00 13.93	A
_	MOTA	938	N	ARG	138	23.616		113.982	1.00 13.99	A
5	ATOM	939	CA	ARG	138	24.061	8.490	115.034	1.00 14.63	A
	ATOM	940	CB	ARG	138	23.520		114.788	1.00 11.07	· A
	MOTA	941	CG	ARG	138	22.026		115.030	1.00 10.07	A
	MOTA	942	CD	ARG	138	21.514		114.706	1.00 12.89	A
10	ATOM	943	NE	ARG	138	20.063		114.816	1.00 14.12	A
10	MOTA MOTA	944 945	CZ	ARG ARG	138	19.395		115.961	1.00 16.84	A
	ATOM	946		ARG	138 138	20.043 18.070		117.123 115.943	1.00 17.01 1.00 16.58	A A
	ATOM	947	C	ARG	138	25.590		115.105	1.00 14.82	A
	MOTA	948	ŏ	ARG	138	26.175		116.189	1.00 17.18	Ä
15	MOTA	949	N	THR	139	26.227		113.943	1.00 13.19	A
	MOTA	950	CA	THR	139	27.676		113.864	1.00 14.27	À
	MOTA	951	CB	THR	139	28.134	8.347	112.394	1.00 15.10	A
	MOTA	952		THR	139	27.671		111.877	1.00 16.74	A
20	MOTA	953		THR	139	29.663		112.290	1.00 15.25	A
20	MOTA	954	Č	THR	139	28.315		114.473	1.00 14.96	A
	MOTA MOTA	955 956	O N	THR LEU	139	. 29.268		115.247	1.00 16.32	A
	ATOM	957	CA	LEU	140 140	27.802 28.374		114.128 114.664	1.00 13.16	A A
	ATOM	958	CB	LEU	140	27.742		113.988	1.00 13.55	A
25	ATOM	959	CG	LEU	140	28.065		112.489	1.00 15.01	·Â
	ATOM	960		LEU	140	27.116		111.824	1.00 15.28	. A
	MOTA	961	CD2	LEU	140	29.535		112.286	1.00 12.18	A
	MOTA	962	C	LEU	140	28.168	12.200	116.165	1.00 14.55	A
20	MOTA	963	0	LEU	140	29.031		116.900	1.00 14.87	A
30	MOTA	964	N	HIS	141	27.021		116.621	1.00 15.53	A
	MOTA	965	CA	HIS	141	26.715		118.041	1.00 15.51	A
	ATOM ATOM	966 967	CB CG	HIS	141	25.241		118.265	1.00 17.50	A
	MOTA	968		HIS	141 . 141	24.809 24.144		119.698 120.400	1.00 19.49 1.00 20.09	A
35	ATOM	969		HIS	141	25.057		120.584	1.00 22.94	A A
	MOTA	970		HIS	141	24.561		121.769	1.00 21.94	A
	MOTA	971		HIŞ	141	24.002		121.683	1.00 21.59	Ä
	ATOM	972	C	HIS	141	27.638		118.787	1.00 14.45	A
40	MOTA	973	0	HIS	141	28.133		119.864	1.00 12.82	A
40	ATOM	974	N	GLN	142	27.893		118.202	1.00 12.87	A
	MOTA	975	CA	GLN	142	28.753		118.852	1.00 14.02	A
	MOTA	976	CB	GLN	142	28.542		118.239	1.00 13.39	A
	MOTA MOTA	977 978	CD	GLN	142	27.299		118.741	1.00 20.05	A
45	MOTA	979		GLN	142 142	27.237 26.660		120.262 120.910	1.00 21.32 1.00 21.37	A A
	MOTA	980		GLN	142	27.850		120.837	1.00 19.74	A
	ATOM	981	C	GLN	142	30.243		118.862	1.00 13.74	Ä
	MOTA	982	0	GLN	142	30.961		119.759	1.00 14.17	A
~^	MOTA	983	N	ILE	143	30.713		117.870	1.00 13.21	A
50	MOTA	984	CA	ILE	143	32.119	10.087	117.826	1.00 13.39	A
	ATOM	985	CB	ILE	143	32.435	10.932		1.00 11.43	A
	ATOM	986		ILE	143	33.847	11.507		1.00 13.15	A
	ATOM ATOM	987 988		ILE	143	32.282	10.068		1.00 9.90	A
55	MOTA	989	CDI	ILE	143 143	32.437 32.454	10.844	119.082	1.00 8.46 1.00 14.99	A
	ATOM	990	ŏ	ILE	143	33.473	10.660		1.00 13.04	A A
	MOTA	991	N	PHE	144	31.581		119.419	1.00 17.68	Ä
	MOTA	992	CA	PHE	144	31.741	12.694		1.00 20.78	A
~	ATOM	993	CB	PHE	144	30.771	13.882		1.00 17.56	A
60	MOTA	994	CG	PHE	144	31.153	14.924	119.549	1.00 18.09	A
	MOTA	995	CD1		144	32.205	15.796		1.00 18.10	A
	ATOM	996	CD2		144	30.492	15.013		1.00 17.52	A
	MOTA	997	CE1		144	32.596	16.740		1.00 19.03	A
65	ATOM	998	CE2		144	30.873	15.949		1.00 16.50	A
J.	MOTA MOTA	999 1000	CZ C	PHE PHE	144 144	31.926 31.481	11.908	117.639	1.00 18.32	A
	ATOM	1000	Ö	PHE	144	32.059	12.203		1.00 24.06 1.00 25.61	A A
	ATOM	1002	N	GLU	145	30.596	10.924		1.00 28.05	Ä
	ATOM	1003	CA	GLU	145	30.270	10.113		1.00 32.18	Ä
70	MOTA	1004	СВ	GLU	145	29.052		122.660	1.00 34.92	A
	MOTA	1005	CG	GLU	145	28.382	8.616	123.877	1.00 41.48	A
	MOTA	1006	CD	GLU	145	27.459		124.604	1.00 46.68	A
	MOTA	1007	OE1	GLU	145	26.808	9.154	125.583	1.00 48.85	A

	•									
•	MOTA	1008	OE2	GLU	145	27.379	10.772	124.205	1.00 48.27	A
	ATOM	1009	С	GLU	145	31.472	9.234	123.300	1.00 33.53	A
	ATOM	1010	ō	GLU	145	31.796		124.465	1.00 35.14	A
5	MOTA	1011	N	LYS	146	32.139		122.272	1.00 33.94	A
J	ATOM	1012	CA	LYS	146	33.289	7.857	122.460	1.00 35.62	A
	ATOM	1013	CB	LYS	146	33.493	6.982	121.218	1.00 35.76	A
	MOTA	1014	CG	LYS	146	32.398	5.949	120.990	1.00 38.40	A
	ATOM	1015	CD	LYS	146	32.750		119.853	1.00 39.00	A
	ATOM									
10		1016	CE	LYS	146	31.822		119.842	1.00 40.55	A
10	ATOM	1017	NZ	LYS	146	32.108	2.871	118.719	1.00 42.99	A
	ATOM	1018	-C	LYS	146	34.600	8.572	122.781	1.00 37.30	A
	ATOM	1019	0	LYS	146	35.279	8.224	123.746	1.00 38.30	A
	MOTA	1020	N	LEU	147	34.959		121.978	1.00 37.75	A
•										
15	MOTA	1021	CA	LEU	147	36.212		122.182	1.00 39.45	A
17	ATOM	1022	CB	LEU	147	36.611		120.894	1.00 36.70	A
	MOTA	1023	CG	LEU	147	36.769	10.134	119.652	1.00 34.99	A
	ATOM	1024	CD1	LEU	147	37.244	10.979	118.483	1.00 32.76	A
	MOTA	1025		LEU	147	37.754		119.940	1.00 33.24	A
	MOTA	1026		LEU	147	36.250		123.355		
20			Č						1.00 41.40	A
20	MOTA	1027	0	LEU	147	37.329		123.803	1.00 41.57	A
	MOTA	1028	N	THR	148	35.091	11.681	123.855	1.00 43.50	A
	ATOM	1029	CA	THR	148	35.078	12.613	124.972	1.00 46.76	A.
	ATOM	1030	CB	THR	148	33.735		125.068	1.00 46.73	A .
	MOTA	1031	OG1		148	33.559		123.901	1.00 45.09	·A
25	ATOM	1032								
25				THR	148	33.717		126.299	1.00 45.59	A
	ATOM	1033	Ç	THR	148	35.327		126.266	1.00 50.09	A
	MOTA	1034	0	THR	148	36.050	12.321	127.149	1.00 50.49	Α
	ATOM	1035	N	ASP	149	34.734	10.660	126.367	1.00 53.41	A
	MOTA	1036	CA	ASP	149	34.899		127.545	1.00 56.45	· A
30	ATOM	1037	CB	ASP	149	34.094		127.395	1.00 57.31	A
		1038								
	MOTA		CG	ASP	149	32.677		127.926	1.00 59.22	A
	ATOM	1039		ASP	149	32.51 9		129.090	1.00 59.37	A
	ATOM	1040	OD2	ASP	149	31.723	8.302	127.191	1.00 59.44	A
	MOTA	1041	С	ASP	149	36.365	9.468	127.778	1.00 57.60	A
35	MOTA	1042	0	ASP	149	36.948		128.800	1.00 57.84	A
	ATOM	1043	N	ASN	150	36.955		126.824		
									1.00 58.66	A
	ATOM	1044	CA	ASN	150	38.354		126.919	1.00 59.63	A
	MOTA	1045	CB	ASN	150	38.699	7.388	125.793	1.00 62.63	A
	MOTA	1046	CG	ASN	150	37.845	6.129	125.832	1.00 65.36	A
40	ATOM	1047	OD1	ASN	150	37.880		126.803	1.00 66.45	A
. •	ATOM	1048		ASN	150	37.070		124.774	1.00 66.13	
										A
	MOTA	1049	C	ASN	150	39.248		126.833	1.00 58.25	A
	MOTA	1050	0	ASN	150	38.814		126.382	1.00 58.50	A
4 ~	MOTA	1051	N	GLY	151	40.492	9.459	127.279	1,.00 56.63	A
45	ATOM	1052	ÇA	GLY	151	41.416	10.579	127.233	1.00 55.03	A
	ATOM	1053	С	GLY	151	41.915		125.820	1.00 53.26	A
	ATOM	1054	ō.	GLY	151	42.983		125.449	1.00 52.83	
		1055	N							A
	MOTA			THR	152	41.149		125.029	1.00 50.83	A
50	MOTA	1056	CA	THR	152	41.519	11.806	123.643	1.00 47.73	A
50	ATOM	1057	СВ	THR	152	40.763	10.858	122.680	1.00 47.39	Α
	ATOM	1058	OG1	THR	152	40.890	9.502	123.127	1.00 48.20	A
	ATOM	1059	CG2	THR	152	41.326	10.975	121.271	1.00 45.61	A
	ATOM	1060	С	THR	152	41.237		123.180	1.00 46.24	A
	ATOM	1061	ŏ	THR	152					
55						40.163		123.425	1.00 46.24	A
22	MOTA	1062	N	GLU	153	42.217		122.510	1.00 43.69	A
	MOTA	1063	CA	GLU	153	42.066	15.165	121.957	1.00 41.25	A
	ATOM	1064	CB	GLU	153	43.386	15.926	122.014	1.00 42.93	A
	MOTA	1065	CG	GLU	153	43.815	16.330	123.407	1.00 46.50	Α.
	MOTA	1066	CD	GLU	153	45.193		123.421	1.00 48.91	A
60	ATOM	1067								
50				GLU	153	46.181		123.196	1.00 49.46	A
	MOTA	1068		GLU	153	45.288	18.177	123.649	1.00 52.22	A
	MOTA	1069	С	GLU	153	41.677	14.898	120.508	1.00 38.96	Α
	ATOM	1070	0	GLU	153	42.232	13.998	119.874	1.00 38.36	Α
	ATOM	1071	N	PHE	154	40.730		119.980	1.00 35.01	A
65	ATOM	1072	CA	PHE	154	40.289				
								118.611	1.00 30.73	A
	MOTA	1073	CB	PHE	154	39.416		118.574	1.00 27.60	A
	MOTA	1074	CG	PHE	154	38.102	14.340	119.282	1.00 24.32	A
	MOTA	1075	CD1	PHE	154	36.965	14.742	118.585	1.00 22.22	A
	MOTA	1076	CD2	PHE	154	38.009		120.652	1.00 24.15	A
70	MOTA	1077		PHE	154	35.751		119.246	1.00 22.43	Ä
	ATOM	1078	CE2		154	36.797				
								121.327	1.00 24.33	A
	MOTA	1079	CZ.	PHE	154	35.664		120.618	1.00 23.63	A
	ATOM	1080	¢	PHE	154	39.498	16.590	118.024	1.00 28.48	A

	MOTA	1081	0	PHE	154	38.921	17.402	118.744	1.00 27.87	A
	MOTA	1082	N	SER	155	39.474		116.702	1.00 26.86	A
	MOTA	1083	CA	SER	155	38.713		116.006	1.00 25.68	A
5	ATOM	1084	CB	SER	155	39.635		115.347	1.00 24.22	A
,	ATOM ATOM	1085 1086	OG	SER	155	. 40.401		114.309	1.00 25.09	A
	ATOM	1087	C	SER SER	155 155	37.920 38.402		114.947 114.380	1.00 26.10 1.00 26.26	A
	ATOM	1088	N	VAL	156	36.697		114.700	1.00 25.25	A A
	ATOM	1089	CA	VAL	156	35.836		113.712	1.00 23.66	Ä
10	ATOM	1090	CB	VAL	156	34.549		114.371	1.00 22.75	Ä
	ATOM	1091		VAL	156	33.671		113.331	1.00 20.72	A
	ATOM	1092	CG2	VAL	156	34.910		115.497	1.00 20.01	A
	MOTA	1093	С	VAL	156	35.447	17.733	112.622	1.00 24.01	A
15	MOTA	1094	0	VAL	156	34.960		112.916	1.00 24.09	A
15	MOTA	1095	N	LYS	157	35.679		111.369	1.00 21.25	Α
	MOTA	1096	CA	LYS	157	35.332		110.220	1.00 20.34	A
	ATOM	1097	CB	LYS	157	36.559		109.347	1.00 24.12	A
	MOTA MOTA	1098 1099	CG CD	LYS	157 157	37.755 37.474		110.028 110.410	1.00 28.05	A
20	ATOM	1100	CE	LYS	157	38.755		110.410	1.00 31.98 1.00 35.17	A A
	ATOM	1101	NZ	LYS	157	39.737		109.726	1.00 35.98	A
	ATOM	1102	c	LYS	157	34.333		109.382	1.00 19.05	Ä
	ATOM	1103	0	LYS	157	34.475		109.209	1.00 18.10	A
0.5	MOTA	1104	N	VAL	158	33.315		108.865	1.00 15.97	A
25	MOTA	1105	CA	VAL	158	32.340		108.025	1.00 14.22	· A
	MOTA	1106	СВ	VAL	158	30.941		108.690	1.00 12.88	. А
	ATOM	1107		VAL	158	31.014		109.931	1.00 10.13	A
	ATOM	1108		VAL	158	30.419		109.031	1.00 13.23	A
30	MOTA MOTA	1109 1110	CO	VAL VAL	158 158	32.221		106.706	1.00 13.72	A
50	ATOM	1111	Ŋ	SER	159	32.469 31.845		106.610	1.00 14.66	A
	ATOM	1112	CA	SER	159	31.702		104.362	1.00 14.88	A A
	ATOM	1113	CB	SER	159	33.034		103.618	1.00 17.14	À
	ATOM	1114	OG	SER	159	32.904		102.279	1.00 23.83	Ä
35	ATOM	1115	С	SER	159	30.609		103.642	1.00 15.89	A
	MOTA	1116	0	SER	159	30.477	15.976	103.822	1.00 15.28	A
	ATOM	1117	N	LEU	160	29.820	17.890	102.838	1.00 15.69	A
	MOTA	1118	CA	LEU	160	28.728		102.098	1.00 15.26	A
40	ATOM	1119	CB	LEU	160	27.388		102.715	1.00 15.28	Ą
40	MOTA	1120	CG	LEU	160	26.121		102.104	1.00 15.37	A
	MOTA MOTA	1121 1122		LEU	160 160	26.236		102.087	1.00 12.97	A
	MOTA	1123	CD2	LEU	160	24.904 28.799		102.904	1.00 14.38	A
	MOTA	1124	ŏ	LEU	160	28.331		100.263	1.00 15.74	A A
45	ATOM	1125	N	LEU	161	29.394	16.822	99.829	1.00 15.44	Ä
	ATOM	1126	CA	LEU	161	29.577	17.052	98.401	1.00 15.04	A
	MOTA	1127	CB	LEU	161	30.923	16.472	97.968	1.00 16.39	Ä
	MOTA	1128	CG	LEU	161	31.753	17.038	96.815	1.00 19.66	A
50	MOTA	1129		LEU	161	32.749	15.955	96.386	1.00 20.66	A
50	ATOM	1130 1131		LEU	161	30.887	17.437	95.641	1.00 20.16	A
	MOTA MOTA	1132	C O	LEU	161 161	28.470 28.200	16.311 15.161	97.680	1.00 15.70	A
	ATOM	1133	N	GLU	162	27.829	16.952	97.989 96.713	1.00 17.10 1.00 15.78	A A
	ATOM	1134	CA	GLU	162	26.763	16.286	95.984	1.00 13.78	A
55	MOTA	1135	СВ	GLU	162	25.413	16.834	96.428	1.00 14.46	A
	MOTA	1136	CG	GLU	162	25.218	16.645	97.928	1.00 17.99	A
	MOTA	1137	CD	GLU	162	23.781	16.776	98.372	1.00 18.53	A
	MOTA	1138		GLU	162	23.532	16.663	99.588	1.00 20.86	A
4۸	ATOM	1139		GLU	162	22.902	16.984	97.513	1.00 17.99	A
60	ATOM	1140	Ç	GLU	162	26.948	16.403	94.489	1.00 12.56	A
	MOTA	1141	0	GLU	162	27.425	17.414	93.985	1.00 12.95	A
	MOTA MOTA	1142	N	ILE	163	26.575	15.346	93.782	1.00 11.75	A
	ATOM	1143 1144	CA CB	ILE ILE	163 163	26.736 27.588	15.303 14.077	92.340 91.941	1.00 11.19	. A
65	ATOM	1145		ILE	163	27.790	14.044	90.436	1.00 10.80 1.00 9.29	· A
	ATOM	1146		ILE	163	28.927	14.121	92.681	1.00 9.29	A A
	ATOM	1147		ILE	163	29.667	12.777	92.718	1.00 10.31	A
	ATOM .	1148	c	ILE	163	25.393	15.238	91.626	1.00 12.19	Ä
-	MOTA	1149	0	ILE	163	24.524	14.441	91.985	1.00 13.50	A
70	MOTA	1150	N	TYR	164	25.228	16.089	90.620	1.00 10.80	A
	MOTA	1151	CA	TYR	164	24.011	16.125	89.826	1.00 11.96	A
	ATOM	1152	CB	TYR	164	23.038	17.194	90.353	1.00 11.56	A
	MOTA	1153	CG	TYR	164	21.746	17.240	89.573	1.00 10.77	A

	MOTA	1154	CD1	TYR	164	21.639	18.005	88.408	1.00 9.75	A
	MOTA	1155		TYR	164	20.479	17.991	87.638	1.00 8.60	A
	MOTA	1156	CD2	TYR	164	20.653	16.457	89.954	1.00 8.92	A
	ATOM	1157	CE2		164					
5						19.483	16.428	89.187		A
3	ATOM	1158	CZ	TYR	164	19.405	17.197	88.031	1.00 10.37	A
	ATOM	1159	ОН	TYR	164	18.264	17.167	87.261	1.00 9.00	A
		1160	C	TYR						
	ATOM				164	24.415	16.443	88.395	1.00 12.68	À
	MOTA	1161	0	TYR	164	25.048	17.468	88.131	1.00 13.49	A
	MOTA	1162	N	ASN	165	24.075	15.550	87.478	1.00 12.65	A
10										
10	MOTA	1163	CA	asn	165	24.410	15.745	86.078	1.00 14.45	A
	MOTA	1164	CB	ASN	165	23.541	16.864	85.515	1.00 18.24	A
	MOTA	1165	CG	ASN	165	23.498	16.869	84.010	1.00 24.46	A
	MOTA	1166		asn	165	23.396	15.817	83.374	1.00 29.01	A
	MOTA	1167	ND2	ASN	165	23.556	18.061	83.422	1.00 27.99	A
15	ATOM	1168	С	ASN	165	25.903	16.069	85.930	1.00 14.74	A
	ATOM	1169	0	ASN	165	26.290	16.972	85.184	1.00 13.82	A
	MOTA	1170	N	GLU	166	26.729	15.321	86.663	1.00 13.32	A
	ATOM	1171	CA	GLU	166	28.178	15.475	86.645	1.00 13.84	A
00	MOTA	1172	CB	GLU	166	28.730	15.118	85.265	1.00 11.37	A
20	MOTA	1173	CG	GLU	166	28.676	13.635	84.952	1.00 13.48	A
	ATOM	1174	CD	GLU	166	29.270	12.781	86.069	1.00 15.85	A
	ATOM	1175		GLU	166	28.518	12.411	86.995	1.00 14.50	Α.
	MOTA	1176	OE2	GLU	166	30.491	12.490	86.022	1.00 14.74	Α
	MOTA	1177	С	GLU	166	28.724	16.835	87.067	1.00 15.33	Ά
25										
23	ATOM	1178	0	GLU	166	29.809	17.229	86.650	1.00 16.01	A
	MOTA	1179	N	GLU	167	27.970	17.555	87.885	1.00 16.84	A
	ATOM	1180	CA	GLU	167	28.415	18.850	88.381	1.00 16.72	A
	MOTA	1181	CB	GLU	167	27.403	19.949	88.052	1.00 19.43	A
	ATOM	1182	CG	GLU	167	27.235	20.216	86.570	1.00 23.50	A
30	ATOM	1183	CD	GLU	167	26.307	21.388	86.309	1.00 28.67	
-										A
	MOTA	1184		GLU	167	25.176	21.382	86.846	1.00 32.20	A
	ATOM	1185	OE2	GLU	167	26.707	22.316	85.571	1.00 31.83	A
	ATOM	1186	С	GLU	167	28.522	18.685	89.888	1.00 15.13	A
25.	MOTA	1187	0	GLU	167	27.773	17.908	90.480	1.00 15.63	A
35 '	MOTA	-1188	N	LEU	168	29.449	19.408	90.501	1.00 12.84	A
	ATOM	1189	CA	LEU	168	29.672	19.312	91.939	1.00 12.94	A
	MOTA	1190	CB	LEU	168	31.171	19.220	92.217	1.00 14.17	A
	MOTA	1191	CG	LEU .	168	31.859	17.853	92.232	1.00 18.45	A
	MOTA	1192	CD1		168	31.289	16.947	91.164	1.00 19.30	A
40										
40	MOTA	1193		LEU	168	33.366	18.058	92.047	1.00 18.21	A
	MOTA	1194	С	LEU	168	29.080	20.467	92.732	1.00 11.51	A
	MOTA	1195	0	LEU	168	29.228	21.631	92.357	1.00 12.03	A
	MOTA	1196	N	PHE	169	28.415	20.138	93.834	1.00 8.76	A
	ATOM	1197	CA	PHE	169	27.812	21.152	94.682	1.00 10.79	A
45	ATOM	1198	CB	PHE	169	26.286	21.155	94.543	1.00 8.69	
										A
	MOTA	1199	CG	PHE	169	25.804	21.329	93.127	1.00 9.29	A
	MOTA	1200	CD1	PHE	169	25.568	20.219	92.314	1.00 8.53	A
	ATOM	1201		PHE	169	25.605	22.595	92.598	1.00 7.95	A
50	MOTA	1202	CE1		169	25.140	20.372	90.996	1.00 9.35	A
50	MOTA	1203	CE2	PHE	169	25.178	22.762	91.284	1.00 7.75	A
	ATOM	1204	CZ	PHE	169	24.945	21.648	90.479	1.00 9.59	A
	MOTA	1205	С	PHE	169	28.187	20.923	96.138	1.00 12.65	. А
	MOTA	1206	0	PHE	169	28.319	19.788	96.593	1.00 13.12	A
	MOTA	1207	N	ASP	170	28.369	22.027	96.850	1.00 12.78	A
55			CA							
55	MOTA	1208		ASP	170	28.724	22.018	98.253	1.00 13.35	A
	ATOM	1209	CB	ASP	170	29.817	23.060	98.502	1.00 12.29	A
	MOTA	1210	CG	ASP	170	30.300	23.072	99.931	1.00 13.08	Α
	MOTA	1211	OD1		170	29.577		100.817	1.00 14.08	Α.
	MOTA	1212	OD2	ASP	170	31.404	23.598	100.176	1.00 15.39	A
60 -	ATOM	1213	С	ASP	170	27.456	22.413	99.001	1.00 15.21	A
	MOTA	1214	0	ASP	170	27.086	23.588	99.003	1.00 13.76	A
	MOTA	1215	N	LEU-	171	26.797	21.445	99.635	1.00 16.64	A
	ATOM	1216	CA	LEU	171	25.563		100.365	1.00 19.47	Ä
4 5	MOTA	1217	CB	LEU	171	24.650		100.376	1.00 18.16	A
65	MOTA	1218	CG	LEU	171	23.677	20.315	99.200	1.00 20.70	A
	MOTA	1219	CD1		171	22.739	21.515	99.130	1.00 21.59	
										A
	ATOM	1220	CD2		171	24.436	20.192	97.900	1.00 19.74	A
	MOTA	1221	С	LEU	171	25.724	22.233	101.794	1.00 21.95	A
	ATOM	1222	Ō	LEU	171	24.747		102.536	1.00 24.93	
70										λ
/U	ATOM	1223	N	LEU	172	26.931	22.618	102.197	1.00 24.33	A
	MOTA	1224	CA	LEU	172	27.108	23,129	103.558	1.00 25.95	Α
	MOTA	1225	CB.	LEU						
					172	28.101		104.353	1.00 22.64	A
	MOTA	1226	CG	LEU	172	27.683	20.835	104.713	1.00 21.08	A

	MOTA	1227	CD1	LEU	172	28.747	20,208	105.584	1.00 19.49	A
	MOTA	1228		LEU	172	26.353	20.821	105.450	1.00 20.02	A
	MOTA	1229	c	LEU	172	27.550		103.579	1.00 28.46	· A
5	MOTA	1230	0	LEU	172	27.222		104.512	1.00 33.47	A
ב	MOTA	1231	N	ASN	173	28.280		102.557	1.00 27.52	A
	ATOM .	1232	CA	ASN	173	28.733	26.404	102.479	1.00 28.63	A
	ATOM	1233	CB	ASN	173	29.491	26.621	101.166	1.00 28.72	A
	MOTA	1234	CG	ASN	173	30.022		101.013	1.00 30.51	A
	MOTA	1235		ASN.	173		28.350		1.00 32.23	A
10										
10	ATOM	1236		ASN	173	29.709		101.969	1.00 31.50	A
	ATOM	1237	С	ASN	173	27.514		102.555	1.00 30.66	· A
	MOTA	1238	0	ASN	173	26.639	27.296	101.688	1.00 30.81	A
	MOTA	1239	N	PRO	174	27.434	28.164	103.602	1.00 32.10	A
	ATOM	1240	CD	PRO	174	28.196		104.862	1.00 32.35	A
15	MOTA	1241	CA	PRO	174	26.298		103.741	1.00 34.00	A
13						26.085		105.243		
	MOTA	1242	CB	PRO	174				1.00 33.56	А
	ATOM	1243	CG	PRO	174	27.500		105.740	1.00 33.25	A
	MOTA	1244	С	PRO	174	26.566 ·	30.469		1.00 35.77	A
	MOTA	1245	0	PRO	174	26.014	31.452	103.667	1.00 38.93	A
20	MOTA	1246	N	SER	175	27.404	30.557	102.155	1.00 36.48	A
	ATOM	1247	CA	SER	175	27.734		101.568	1.00 36.56	A
	ATOM	1248	CB	SER	175	29.104		102.064	1.00 36.53	A
	ATOM	1249	OG	SER	175	29.142		103.481	1.00 38.61	A
25	MOTA	1250	С	SER	175	27.746		100.059	1.00 36.99	A
25	ATOM	1251	0	SER	175	28.234	32.639	99.366	1.00 37.49	A
	MOTA	1252	N	SER	176	27.226	30.631	99.560	1.00 37.22	. A
	ATOM	1253	CA	SER	176	27.142	30.385	98.125	1.00 38.02	A
	ATOM	1254	CB	SER	176	28.296	29.483	97.662	1.00 37.78	A
		1255	OG	SER	176	28.200	28.177	98.213	1.00 37.44	Ä
30	ATOM									
20	ATOM	1256	C	SER	176	25.807	29.699	97.862	1.00 37.53	A
	MOTA	1257	0	SER	176	25.277	29.016	98.734	1.00 37.34	A
	MOTA	1258	N	ASP	177	25.248	29.891	96.676	1.00 38.02	A
	ATOM	1259	CA	ASP	177	23.983	29.243	96.366	1.00 39.18	A
	ATOM	1260	CB	ASP	177	23.012	30.229	95.704	1.00 41.03	A
35	ATOM	1261	CG	ASP	177	23.585	30.879	94.466	1.00 42.23	A
JJ	ATOM	1262	OD1		177	23.936	30.156	93.511	1.00 43.11	Ä
	MOTA	1263	OD2		177	23.679	32.122	94.447	1.00 44.29	A
	ATOM	1264	С	ASP	177	24.219	28.031	95.471	1.00 38.57	A
	ATOM	1265	0	ASP	177	25.274	27.910	94.849	1.00 37.31	A
40	ATOM	1266	N	VAL	178	23.232	27.141	95.415	1.00 38.30	A.
. •	MOTA	1267	CA	VAL	178	23.329	25.918	94.626	1.00 38.53	A
	ATOM	1268	CB	VAL	178	22.091	25.018	94.830	1.00 38.67	A
			CG1		178			96.266		
	MOTA	1269				22.040	24.532		1.00 38.55	A
45	ATOM	1270	CG2		178	20.828	25.780	94.472	1.00 38.63	A
45	MOTA	1271	С	VAL	178	23.526	26.111	93.129	1.00 38.49	A
	MOTA	1272	0	VAL	178	23.589	25.138	92.385	1.00 39.24	A
	ATOM	1273	N	SER	179	23.618	27.357	92.683	1.00 38.10	A
	ATOM	1274	CA	SER	179	23.823	27.626	91.268	1.00 37.56	A
	MOTA	1275	CB	SER	179	23.265	29.000	90.905	1.00 39.68	A
50										
20	MOTA	1276	OG	SER	179	21.942	29.155	91.390	1.00 45.54	A
	MOTA	1277	C	SER	179	25.318	27.594	90.981	1.00 36.56	A
	MOTA	1278	0	SER	179	25.740	27.516	89.828	1.00 37.57	A
	ATOM	1279	N	GLU	180	26.112	27.663	92.044	1.00 34.30	A
	MOTA	1280	CA	GLU	180	27.566	27.651	91.938	1.00 34.69	A
55	MOTA	1281	CB	GLU	180	28.173	28.564	93.018	1.00 36.86	A
	ATOM	1282	CG	GLU .	180	27.906	30.055	92.767	1.00 41.33	Ä
		1283			180					
	АТОМ		CD	GLU		28.262	30.958	93.945	1.00 42.95	A
	ATOM	1284	OE1		180	27.629	30.832	95.017	1.00 43.98	A
	MOTA	1285	OE2	GLU	180	29.174	31.798	93.795	1.00 44.03	A
60	MOTA	1286	С	GLU	180	28.147	26.241	92.048	1.00 32.62	A
	MOTA	1287	0	GLU	180	28.084	25.614	93.104	1.00 31.99	A
	MOTA	1288	N	ARG	181	28.706	25.745	90.951	1.00 30.63	A
			CA	ARG	181		24.415	90.941	1.00 30.51	
	MOTA	1289				29.292				A
45	MOTA	1290	CB	ARG	181	29.050	23.739	89.587	1.00 34.25	À
65	MOTA	1291	CG	ARG	181	29.575	24.493	88.379	1.00 40.52	A
	MOTA	1292	CD	ARG	181	29.025	23.901	87.069	1.00 46.73	A
	MOTA	1293	NE	ARG	181	29.587	22.592	86.721	1.00 50.11	A
	MOTA	1294	cz	ARG	181	30.818	22.400	86.251	1.00 52.44	A
	MOTA	1295	NH1		181		23.435	86.070	1.00 53.59	
70										A
70	MOTA	1296	NH2		181	31.236	21.173	85.951	1.00 52.52	A
	MOTA	1297	Ċ	ARG	181	30.781	24.480	91.249	1.00 28.82	A
	ATOM	1298	0	ARG	181	31.438	25.483	90.979	1.00 29.29	A
	MOTA	1299	N	LEU	182	31.308	23.408	91.829	1.00 25.57	A

										•
•	MOTA	1300	CA	LEU	182	32.718	23.348	92.182	1.00 21.92	A
	MOTA	1301	CB	LEU	182	32.899	22.553	93.471	1.00 20.02	A
	ATOM	1302	CG	LEU	182	32.155	23.087	94.700	1.00 20.20	A
_	MOTA	1303		LEU	182	32.161	22.044	95.812	1.00 17.99	A
5	MOTA	1304	CD2	LEU	182	32.802	24.379	95.159	1.00 16.82	A
	ATOM	1305	С	LEU	182	33.515	22.696	91.069	1.00 22.08	A
	ATOM	1306	0	LEU	182	32.960	21.949	90.257	1.00 19.82	A
						34.814	23.000	91.028	1.00 22.61	
	MOTA	1307	N	GLN	183					A
10	MOTA	1308	CA	GLN	183	35.726	22.435	90.034	1.00 20.55	A
10	MOTA	1309	CB	GLN	183	36.702	23.488	89.523	1.00 22.39	A
	MOTA	1310	·CG	GLN	183	36.100	24.557	88.652	1.00 28.44	A
	ATOM	1311	CD	GLN	183	36.981	25.799	88.593	1.00 32.88	A
•	MOTA	1312		GLN	183	37.054	26.572	89.557	1.00 34.28	A
	MOTA	1313	NE2	GLN	183	37.664	25.989	87.468	1.00 33.10	A
15	MOTA	1314	С	GLN	183	36.518	21.327	90.702	1.00 19.22	A
	MOTA	1315	0	GLN	183	36.795	21.390	91.897	1.00 18.40	A
•	ATOM	1316	N	MET	184	36.902	20.330	89.915	1.00 18.69	A
	MOTA	1317	CA	MET	184	37.646	19.191	90.416	1.00 19.64	A
^^	MOTA	1318	CB	MET	184	36.747	17.951	90.361	1.00 21.90	A
20	MOTA	1319	CG	MET	184	37.304	16.701	91.011	1.00 25.13	Α
	MOTA	1320	SD	MET	184	36.147	15.306	90.921	1.00 31.12	A
	ATOM	1321	CE	MET	184	36.591	14.620	89.352	1.00 23.65	À.
	MOTA	1322	C	MET	184	38.897	18.983	89.568	1.00 21.60	A
	MOTA	1323	0	MET	184	38.840	19.035	88.341	1.00 21.33	A
25	MOTA	1324	N	PHE	185	40.026	18.750	90.230	1.00 23.48	Α
	MOTA	1325	CA	PHE	185	41.299	18.531	89.544	1.00 25.16	A
									1.00 25.59	
	MOTA	1326	CB	PHE	185	42,231	19.736	89.709		A
	MOTA	1327	CG	PHE	185	41.595	21.064	89.414	1.00 25.42	A
••	ATOM	1328	CD1	PHE	185	40.791	21.691	90.360	1.00 23.63	A
30	MOTA	1329	CD2	PHE	185	41.857	21.718	88.211	1.00 26.39	A
	MOTA	1330	CE1		185	40.261	22.956	90.124	1.00 24.23	A
							22.987			
	MOTA	1331	CE2	PHE	185	41.332		87.961	1.00 27.17	A
	MOTA	1332	CZ	PHE	185	40.533	23.609	88.921	1.00 25.70	A
	MOTA	1333	С	PHE	185	42.002	17.326	90.149	1.00 26.03	A
35	ATOM	1334	0	PHE	185	41.709	16.937	91.275	1.00 25.54	A
	ATOM	1335	N	ASP	186	42.941	16.743	89.414	1.00 29.33	A
	MOTA	1336	CA	ASP	186	43.692	15.603	89.930	1.00 33.38	A
	MOTA	1337	CB	ASP	186	44.461	14.913	88.801	1.00 35.26	A
	ATOM	1338	CG	ASP	186	43.546	14.212	87.816	1.00 37.12	A
40	MOTA	1339		ASP	186	43.644	14.505		1.00 37.66	A
	ATOM	1340	OD2		186	42.733	13.368	88.257	1.00 36.31	A
	MOTA	1341	С	ASP	186	44.675	16.117	90.977	1.00 35.30	A
	MOTA	1342	0	ASP	186	45.167	17.238	90.865	1.00 35.53	A
	MOTA	1343	N	ASP	187	44.959	15.313	91.996	1.00 38.26	A
45	MOTA	1344	CA	ASP	187	45.890	15.739	93.037	1.00 43.31	A
	MOTA	1345	СВ	ASP	187	45.489	15.138	94.385	1.00 42.12	A
	MOTA	1346	CG	ASP	187	46.217	15.784	95.546	1.00 42.51	A
	MOTA	1347	OD1	ASP	187	45.755	15.631	96.696	1.00 42.87	A
	MOTA	1348	OD2	ASP	187	47.252	16.442	95.307	1.00 41.23	A
50	MOTA	1349	С	ASP	187	47.307	15.318	92.665	1.00 46.67	A
	ATOM	1350	ō	ASP	187	47.644	14.138	92.719	1.00 48.15	A
									1.00 50.27	
	MOTA	1351	N	PRO	188	48.160	16.283	92.286		A
	MOTA	1352	CD	PRO	188	47.945	17.735	92.408	1.00 50.91	A
	ATOM	1353	ÇA	PRO	188	49.548	15.996	91.897	1.00 53.10	A
55	MOTA	1354	СВ	PRO	188	50.107	17.376	91.561	1.00 52.20	A
	MOTA	1355	CG	PRO	188	49.364	18.263	92.503	1.00 52.65	A
	MOTA	1356	C	PRO	188	50.366	15.279	92.966	1.00 55.80	A
	MOTA	1357	0	PRO	188	51.319	14.568	92.650	1.00 56.91	Α.
	MOTA	1358	N	ARG	189	49.996	15.466	94.228	1.00 58.59	A
60	MOTA	1359	CA	ARG	189	50.703	14.812	95.321	1.00 61.67	A
	ATOM	1360	СВ	ARG	189	50.294	15.428	96.658	1.00 63.13	A
	MOTA	1361	CG	ARG	189	50.839	16.823	96.881	1.00 65.91	A
	MOTA	1362	CD	ARG	189	50.181	17.468	98.083	1.00 68.55	A
	ATOM	1363	NE	ARG	189	48.754	17.670	97.855	1.00 70.63	Α
65	MOTA	1364	CZ	ARG	189	47.906	18.095	98.784	1.00 72.05	A
	MOTA	1365	NH1	ARG	189	48.340	18.362	100.010	1.00 72.50	A
	MOTA	1366	NH2		189	46.623	18.252	98.484	1.00 72.44	A
	MOTA	1367	С	ARG	189	50.402	13.316	95.321	1.00 63.14	A
	ATOM	1368	0	ARG	189	51.085	12.537	94.652	1.00 63.21	A
70	MOTA	1369	N	ASN	190	49.377	12.916	96.070	1.00 64.30	A
. •	MOTA	1370	CA	ASN	190	49.000	11.509	96.140	1.00 65.20	A
	MOTA	1371	CB	ASN	190	48.225	11.220	97.439	1.00 66.56	A
	MOTA	1372	CG	ASN	190	47.172	12.273	97.753	1.00 67.73	A

	ATOM	1373	OD1	ASN	190	47.491	13.443	97.982	1.00 67.83	A
	ATOM	1374		ASN	190	45.909	11.858	97.773	1.00 67.20	A
	ATOM	1375	C	ASN	190	48.197	11.061	94.918	1.00 64.94	A
									1.00 64.53	
5	MOTA	1376	0	ASN	190	47.182	11.662	94.565		A
)	MOTA	1377	N	LYS	191	48.669	9.999	94.273	1.00 64.72	A
	MOTA	1378	CA	LYS	191	48.018	9.463	93.083	1.00 63.98	A
	MOTA	1379	CB	LYS	191	48.810	8.266	92.541	1.00 65.18	A
	. ATOM	1380	CG	LYS	191	48.799	7.041	93.447	1.00 66.13	A
	MOTA	1381	CD	LYS	191	49.405	5.830	92.747	1.00 67.02	A
10	MOTA	1382	CE	LYS	191	49.274	4.572	93.593	1.00 68.29	A
	MOTA	1383	NZ	LYS	191	49.860	3.375	92.919	1.00 69.29	· A
	MOTA	1384	С	LYS	191	46.577	9.039	93.358	1.00 62.26	A
	MOTA	1385	ŏ	LYS	191	46.151	8.963	94.513	1.00 63.17	A
	MOTA	1386	N	ARG	192	45.843	8.756	92.282	1.00 58.36	A
15	MOTA	1387	CA	ARG	192	44.440	8.350	92.348	1.00 54.26	Ä
13	ATOM	1388	CB	ARG	192	44.308	6.833	92.578	1.00 56.88	Ä
					192					•
	ATOM	1389	CG	ARG		44.776	6.289	93.926	1.00 59.69	A
	MOTA	1390	CD	ARG	192	43.939	5.062	94.306	1.00 62.18	A
20	MOTA	1391	NE	ARG	192	44.633	4.121	95.181	1.00 64.60	A
20	MOTA	1392	CZ	ARG	192	45.640	3.344	94.792	1.00 66.61	A
	MOTA	1393	NH1	ARG	192	46.074	3.400	93.539	1.00 66.97	A
	MOTA	1394	NH2	ARG	192	46.209	2.505	95.650	1.00 67.30	A
	MOTA	1395	С	ARG	192	43.619	9.106	93.391	1.00 50.08	A
	MOTA	1396	0	ARG	192	42.742	8.538	94.049	1.00 50.87	A
25	ATOM	1397	N	GLY	193	43.909	10.395	93.531	1.00 44.14	A
	ATOM	1398	CA	GLY	193	43.183	11.231	94.469	1.00 35.61	A
	MOTA	1399		GLY	193	42.799	12.482	93.712	1.00 30.34	A
	ATOM	1400	ō	GLY	193	43.343	12.732	92.639	1.00 30.32	A
	ATOM	1401	N	VAL	194	41.865	13.264	94.238	1.00 25.49	Ä
30	ATOM	1402	CA	VAL	194	41.463	14.489	93.557	1.00 21.22	A
-	MOTA	1403	CB	VAL	194	40.078	14.359	92.884	1.00 20.31	Ä
	ATOM	1404	CG1	VAL	194	40.100	13.289	91.809	1.00 19.29	
				VAL		39.032		93.935		A
	MOTA	1405			194		14.059		1.00 18.96	A
35	ATOM	1406	C	VAL	194	41.375	15.668	94.505	1.00 20.08	A
33	MOTA	1407	0	VAL	194	41.417	15.515	95.722	1.00 20.27	Α.
	MOTA	1408	N	ILE	195	41.238	16.853	93.930	1.00 20.12	A
	ATOM	1409	CA	ILE	195	41.109	18.065	94.713	1.00 18.57	A
	MOTA	1410	СВ	ILE	195	42.298	19.014	94.477	1.00 20.69	A
in	MOTA	1411	CG2	ILE	195	42.011	20.362	95.118	1.00 21.74	A
40	MOTA	1412	CG1	ILE	195	43.584	18.392	95.029	1.00 21.99	A
	MOTA	1413	CD1	ILE	195	44.853	19.212	94.722	1.00 23.27	, A
	ATOM	1414	С	ILE	195	39.838	18.791	94.297	1.00 17.41	A
	ATOM	1415	0	ILE	195	39.639	19.077	93.115	1.00 15.50	A
	ATOM	1416	N	ILE	196	38.962	19.066	95.256	1.00 17.01	. А
45	MOTA	1417	CA	ILE	196	37.751	19.805	94.939	1.00 18.54	A
	MOTA	1418	CB	ILE	196	36.493	19.251	95.639	1.00 18.28	A
	MOTA	1419		ILE	196	35.299	20.143	95.314	1.00 13.69	Ä
	MOTA	1420	CG1	ILE	196	36.209	17.819	95.171	1.00 17.38	Ä
		1421	CD1		196	37.016		95.894		
50	MOTA						16.775		1.00 21.62	A
50	MOTA	1422	C	ILE	196	37.981	21.232	95.407	1.00 20:22	A
	MOTA	1423	0	ILE	196	38.001	21.517	96.606	1.00 20.32	A
	MOTA	1424	N	LYS	197	38.158	22.122	94.441	1.00 21.72	A
	MOTA	1425	CA	LYS	197	38.418	23.524	94.709	1.00 23.72	A
E E	ATOM	1426	CB	LYS	197	38.807	24.209	93.397	1.00 26.40	A
55	ATOM	1427	CG	LYS	197	39.068	25.693	93.481	1.00 29.01	Α
	MOTA	1428	CD	LYS	197	39.519	26.211	92.125	1.00 32.62	A
	MOTA	1429	CE	LYS	197	39.538	27.728	92.088	1.00 33.50	A
	MOTA	1430	NZ	LYS	197	38.172	28.259	92.341	1.00 36.03	A
	ATOM	1431	C	LYS	197	37.226	24.225	95.348	1.00 24.04	A
60	MOTA	1432	0	LYS	197	36.139	24.261	94.782	1.00 24.54	A
	MOTA	1433	N	GLY	198	37.436	24.763	96.543	1.00 24.46	A
	ATOM	1434	CA	GLY	198	36.377	25.478	97.227	1.00 25.68	A
	MOTA	1435	c	GLY	198	35.413	24.681	98.088	1.00 26.82	A.
	MOTA	1436	ò	GLY	198	34.482	25.256	98.652	1.00 27.32	À
65	MOTA	1437	N	LEU	199	35.612	23.230	98.202	1.00 27.32	
55					199					A
	MOTA	1438	CA	LEU		34.714	22.558	99.017	1.00 27.19	A
	ATOM	1439	CB	LEU	199	35.008	21.068	98.819	1.00 26.21	A
	MOTA	1440	CG	LEU	199	33.908	20.008	99.023	1.00 27.04	A
70	ATOM	1441		LEU	199	34.563	18.778	99.630	1.00 25.53	A
70	ATOM	1442		LEU	199	32.779	20.497	99.924	1.00 24.18	A
	ATOM	1443	Ç	LEU	199	34.920		100.484	1.00 27.51	A
	MOTA	1444	0	LEU	199	36.024		101.005	1.00 28.57	A
	MOTA	1445	N	GLU	200	33.856	23.346	101.150	1.00 28.60	A

	ATOM	1446	CA	GLU	200	33.950	23.721 1	02 553	1.00 31.25	A
	MOTA	1447	CB	GLU	200	32.788	24.644 1	02.935	1.00 34.22	A
	MOTA	1448	CG	GLU	200	32.933	26.067 1	02.419	1.00 39.68	A
		1449	CD	GLU	200	34.051	26.823 1		1.00 42.07	A
_	ATOM									
5	MOTA	1450	OE1	GLU	200	33.921	27.118 1	04.317	1.00 44.27	A
	ATOM	1451	OE2	GLU	200	35.065	27.120 1	02.443	1.00 44.71	Α
									1.00 30.44	
	ATOM	1452	С	GLU	200	33.986	22.540 1			A
	MOTA	1453	0	GLU	200	33.381	21.497 1	03.282	1.00 28.54	A
	MOTA	1454	N	GLU	201	34.716	22.729 1	04 606	1.00 30.76	A
10										
10	MOTA	1455	CA	GLU	201	34.841	21.730 1	05.649	1.00 29.99	A
	MOTA	1456	CB	GLU	201	36.281	21.247 1	05.742	1.00 29.82	A
									1.00 32.15	
	MOTA	1457	CG	GLU	201	36.755	20.516 1			A
	MOTA	1458	CD	GLU	201	. 38.156	19.977 1	04.676	1.00 35.25	A
	MOTA	1459	OE1	GLU	201	38.408	19.298 1	05 699	1.00 34.69	A
15										
15	ATOM	1460	OE2	GLU	201	39.000	20.227 1	03.786	1.00 36.53	A
	MOTA	1461	С	GLU	201	34.439	22.418 1	06.943	1.00 29.40	A
•							23.248 1		1.00 30.31	Ä
	ATOM	1462	0	GLU	201	35.183				
	MOTA	1463	N	ILE	202	33.256	22.089 1	07.449	1.00 27.91	A
	ATOM	1464	CA	ILE	202	32.765	22.694 1	08 679	1.00 25.94	A
20										
20	MOTA	1465	CB	ILE	202	31.207	22.720 1		1.00 27.58	. А
	ATOM	1466	CG2	ILE	202	30.721	23.125 1	10.096	1.00 24.19	A
	MOTA	1467		ILE	202	30.662	23.706 1	07 682	1.00 28.28	A
	MOTA	1468	CD1	ILE	202	30.809	23.241 1	06.256	1.00 30.78	A
	MOTA	1469	С	ILE	202	33.277	21.932 1	09.889	1.00 25.41	·A
25	ATOM								1.00 25.37	
25		1470	0	ILE	202	33.195	20.703 1			A
	MOTA	1471	N	THR	203	33.811	22.667 1	10.856	1.00 23.88	A
	MOTA	1472	CA	THR	203	34.321	22.070 1	12 083	1.00 22.88	A
	ATOM	1473	CB	THR	203	35.397	22.981 1		1.00 22.77	A
	ATOM	1474	OG1	THR	203	36.542	23.064 1	11.883	1.00 23.19	A
30	MOTA	1475	CG2	THR	203	35.813	22.441 1		1.00 19.08	A
50										
	MOTA	1476	С	THR	203	33.143	21.919 1	13.038	1.00 22.21	A
	MOTA	1477	0	THR	203	32.385	22.867 1	13.242	1.00 22.47	A
•		1478	Ň	VAL	204	32.977	20.728 1		1.00 21.39	À
	MOTA									
	MOTA	1479	CA	VAL	204	31.891	20.474 1	14.549	1.00 21.47	A
35	MOTA	1480	CB	VAL	204	31.248	19.102 1	14.278	1.00 20.28	A
	MOTA	1481		VAL	204	30.034	18.906 1		1.00 21.96	A
	MOTA	1482	CG2	VAL	204	30.859	19.000 1	12.820	1.00 20.66	A
	MOTA	1483	С	VAL	204	32.531	20.490 1	15.939	1.00 23.52	A
		1484		VAL	204	33.083	19.484 1		1.00 24.43	A
40	MOTA		0							
40	MOTA	1485	N	HIS	205	32.468	21.635 1	16.615	1.00 23.51	A
	MOTA	1486	CA	HIS	205	33.088	21.782 1	17.933	1.00 24.78	A
			CB						1.00 24.16	A
	MOTA	1487		HIS	205	32.979	23.238 1			
	ATOM	1488	CG	HIS	205	33.597	24.220 1	17.460	1.00 28.16	A
	ATOM	1489	CD2	HIS	205	34.887	24.595 1	17.281	1.00 28.25	A
45		-			205				1.00 29.05	A
73	MOTA	1490		HIS		32.870	24.885 1			
	MOTA	1491	CEl	HIS	205	33.684	25.623 1	15.759	1.00 27.33	A
	MOTA	1492	NE2	HIS	205	34.914	25.464 1	16.216	1.00 28.33	A
		1493		HIS			20.836 1		1.00 24.15	A
	MOTA		C .		. 205	32.586				
	MOTA	1494	0	HIS	205	33.341	20.445 1	19.909	1.00 24.11	A
50	MOTA	1495	N	ASN	206	31.318	20.458 1	18.945	1.00 25.62	A
-				ASN						
	MOTA	1496	CA		206	30.758	19.552 1		1.00 26.43	A
	ATOM	1497	СB	ASN	206 .	30.598	20, 275 1	21.281	1.00 25.52	A
	ATOM	1498	CG	ASN	206	29.689	21.488 1		1.00 26.18	A
~ ~	MOTA	1499		ASN	206	28.498	21.358 1	20.906	1.00 28.63	A
55	MOTA	1500	ND2	ASN	206	30.246	22.671 1	21.414	1.00 24.14	A
	MOTA	1501	c	ASN		29.422	18.960 1		1.00 27.20	A
	MOTA	1502	0	ASN	206	28.804	19.416 1		1.00 27.37	A
	MOTA	1503	N	LYS	207	28.993	17.933 1	20.212	1.00 27.93	A
40	MOTA	1504	CA	LYS	207	27.751	17.243 1		1.00 30.13	A
60	ATOM	1505	CB.	LYS	207	27.449	16.252 1	21.060	1.00 32.58	A
	MOTA	1506	CG	LYS	207	26.151	15.481 1		1.00 36.84	A
	MOTA	1507	CD	LYS	207	25.112	15.921 1		1.00 40.39	A
	MOTA	1508	CE	LYS	207	25.525	15.543 1	23.349	1.00 41.61	A
	MOTA	1509	NZ	LYS	207	24.489	15.948 1		1.00 43.85	A
65										
O)	MOTA	1510	С	LYS	207	26.571	18.196 1	19.725	1.00 29.76	A
	MOTA	1511	0	LYS	207	25.738	17.972 1	18.850	1.00 30.05	A
									1.00 28.95	
	MOTA	1512	N	ASP	208	26.505	19.260 1			A
	MOTA	1513	CA	ASP	208	25.402	20.214 1	20.429	1.00 27.71	A
	ATOM	1514	CB	ASP	208	25.280	20.981 1		1.00 28.92	A
70										
70	MOTA	1515	CG	ASP	208	24.772	20.093 1		1.00 33.21	, A
	MOTA	1516	OD1	ASP	208	24.967	20.444 1	24.081	1.00 32.92	A
	MOTA	1517		ASP	208	24.165	19.037 1		1.00 34.60	A
	MOTA	1518	С	ASP	208	25.524	21.169 1	19.240	1.00 26.33	A

			_						_
	ATOM	1519	0	ASP	208	24.836	22.186 119.156	1.00 26.39	A
	ATOM	1520	N	GLU	209	26.381	20.810 118.296	1.00 24.27	A
	MOTA	1521	CA	GLU	209	26.580	21.630 117.116	1.00 21.87	A
	MOTA	1522	CB	GLU	209	28.039	22.074 117.066	1.00 23.60	A
5	ATOM	1523	CG	GLU	209	28.331	23.202 116.106	1.00 25.30	A
•		1524	CD	GLU	209	29.678	23.849 116.384	1.00 25.66	. A
	MOTA								
	MOTA	1525	OE1		209	29.872	24.362 117.507	1.00 25.63	A
	MOTA	1526	OE2		209	30.538	23.845 115.481	1.00 26.97	A
	MOTA	1527	С	GLU	209	26.217	20.819 115.874	1.00 19.67	A
10	MOTA	1528	0	GLU	209	26.125	21.350 114.769	1.00 18.53	A
	MOTA	1529	N	VAL	210	25.988	19.528 116.075	1.00 16.60	· A
	MOTA	1530	CA	VAL	210	25.648	18.625 114.985	1.00 17.06	A
								1.00 17.27	
	MOTA	1531	CB	VAL	210	25.654	17.148 115.479		A
16	MOTA	1532	CG1		210	25.307	16.224 114.330	1.00 18.17	A
15	MOTA	1533	CG2	VAL	210	27.028	16.779 116.068	1.00 17.55	A
	MOTA	1534	С	VAL	210	24.305	18.895 114.270	1.00 16.45	A
	ATOM	1535	0	VAL	210	24.267	19.119 113.063	1.00 17.67	A
	MOTA	1536	N	TYR	211	23.203	18.882 115.003	1.00 14.85	A
	ATOM	1537	CA	TYR	211	21.911	19.072 114.366	1.00 15.99	A
20									
20	MOTA	1538	CB	TYR	211	20.789	19.050 115.404	1.00 14.76	A
	MOTA	1539	CG	TYR	211	19.431	18.850 114.780	1.00 14.73	A
	MOTA .	1540	CD1		211	19.179	17.755 113.953	1.00 12.63	A
	MOTA	1541	CE1	TYR	211	17.923	17.557 113.387	1.00 14.15	A
	MOTA	1542	CD2	TYR	211	18.395	19.746 115.025	1.00 15.52	A
25	ATOM	1543	CE2	TYR	211	17.136	19.559 114.466	1.00 16.40	· A
	ATOM	1544	cz	TYR	211	16.903	18.462 113.649		. A
		1545							
	ATOM			TYR	211	15.645	18.271 113.116	1.00 12.99	A
	MOTA	1546	С	TYR	211	21.763	20.303 113.483	1.00 15.43	A
~~	MOTA	1547	0	TYR	211	21.220	20.207 112.383	1.00 17.14	A
30	MOTA	1548	N	GLN	212	22.238	21.456 113.925	1.00 15.05	A
	ATOM	1549	CA	GLN	212	22.080	22.624 113.081	1.00 17.00	A
	ATOM	1550	CB	GLN	212	22.384	23.912 113.855	1.00 18.93	. A
	MOTA	1551	CG	GLN	212	23.803	24.099 114.319	1.00 25.15	A
35	MOTA	1552	CD	GLN	212	23.892	25.178 115.379	1.00 29.02	A
23	MOTA	1553	OE1		212	23.354	26.276 115.209	1.00 30.43	A
	MOTA	1554	NE2	GLN	212	24.562	24.870 116.486	1.00 30.19	A
	MOTA	1555	С	GLN	212	22.903	22.543 111.799	1.00 16.71	A
	MOTA	1556	0	GLN	212	22.459	23.030 110.749	1.00 16.05	A
	ATOM	1557	N	ILE	213	24.077	21.913 111.865	1.00 14.80	A
40	MOTA	1558	CA	ILE	213	24.921	21.776 110.678	1.00 13.74	À
		1559		ILE					
	MOTA		CB		213	26.309	21.148 111.036	1.00 14.83	A
	MOTA	1560	CG2		213	27.118	20.846 109.764	1.00 11.99	A
	MOTA	1561	CG1	ILE	213	27.099	22.122 111.926	1.00 13.49	A
	ATOM	1562	CD1	ILE	213	28.495	21.607 112.366	1.00 12.70	Α
45	MOTA	1563	С	ILE	213	24.170	20.909 109.662	1.00 14.25	A
_	ATOM	1564	Ō	ILE	213	24.135	21.223 108.474	1.00 14.16	A
	ATOM	1565	N	LEU	214	23.546	19.838 110.142	1.00 12.87	A
		1566	CA	LEU				1.00 12.37	
	MOTA				214	22.778	18.968 109.273		A
50	MOTA	1567	CB	LEU	214	22.355	17.705 110.022	1.00 11.53	A
50	MOTA	1568	CG	LEU	214	23.467	16.843 110.623	1.00 10.45	A
	MOTA	1569	CD1	LEU	214	22.840	15.626 111.257	1.00 10.08	A
	ATOM	1570	CD2	LEU	214	24.454	16.418 109.552	1.00 9.12	A
	MOTA	1571	С	LEU	214	21.536	19.695 108.749	1.00 16.52	A
	MOTA	1572	ō	LEU	214	21.172	19.527 107.591	1.00 19.62	A
55		1573	N	GLU			20.495 109.590	1.00 16.71	A
55	MOTA				215	20.881			
	MOTA	1574	CA	GLU	215	19.690	21.239 109.152	1.00 19.78	A
	MOTA	1575	CB	GLU	215	19.085	22.053 110.306	1.00 19.90	A
	MOTA	1576	CG	GLU	215	18.435	21.249 111.418	1.00 21.54	A
	MOTA	1577	CD	GLU	215	17.901	22.154 112.513	1.00 24.54	A
60	MOTA	1578	OE1		215	16.661	22.267 112.659	1.00 25.81	A
••	MOTA	1579		GLU	215	18.728	22.768 113.219	1.00 23.71	
									A
	MOTA	1580	C	GLU	215	20.049	22.211 108.025	1.00 20.52	A
	MOTA	1581	0	GLU	215	19.311	22.361 107.048	1.00 19.08	A
	MOTA	1582	N	LYS	216	21.189	22.878 108.189	1.00 21.26	A
65	ATOM	1583	CA	LYS	216	21.677	23.840 107.215	1.00 22.33	A
	MOTA	1584	СВ	LYS	216	23.046	24.367 107.656	1.00 24.51	A
	ATOM	1585	CG	LYS	216	23.510	25.619 106.938	1.00 28.98	A
	ATOM	1586	CD	LYS	216	.22.872	26.865 107.523	1.00 23.33	Â
70	MOTA	1587	CE	LYS	216	23.331	27.078 108.959	1.00 35.90	Α
/υ	MOTA	1588	NZ	LYS	216	24.819	27.142 109.072	1.00 37.29	A
	ATOM	1589	С	LYS	216	21.782	23.150 105.850	1.00 22.36	A
	ATOM	1590	0	LYS	216	21.371	23.708 104.832	1.00 23.95	A
	MOTA	1591	N	GLY	217	22.318	21.931 105.838	1.00 20.62	A
		-							

	ATOM	1592	CA	GLY	217	22.458	21.193 104	. 595	1.00 19	.15	A
	ATOM	1593	C	GLY	217	21.119	20.836 103		1.00 19		A
	MOTA	1594	0	GLY	217	20.938	20.932 102		1.00 18		A
_	MOTA	1595	N	ALA	218	20.168	20.431 104	.812	1.00 17	.10	A
5	MOTA	1596	CA	ALA	218	18.845	20.070 104	.330	1.00 15	- 84	Α
_	MOTA	1597	CB	ALA	218	17.996	19.525 105		1.00 14		A
	MOTA	1598	С	ALA	218	18.157	21.275 103		1.00 15		A
	MOTA	1599	0	ALA	218	17.533	21.155 102	. 638	1.00 15	.90	A
	MOTA	1600	N	ALA	219	18.273	22.436 104	. 331	1.00 14	.41	Α
10	MOTA	1601	CA	ALA	219	17.638	23.642 103		1.00 14		A
10											
	MOTA	1602	CB	ALA	219	17.776	24.799 104		1.00 12		A
	MOTA	1603	С	ALA	219	18.208	24.051 102	. 452	1.00 13	.46	A
	MOTA	1604	0	ALA	219	17.469	24.441 101	. 561	1.00 13	.70	A
	MOTA	1605	N	LYS	220	19.525	23.978 102		1.00 13	.95	A
15	ATOM	1606	CA	LYS	220	20.146	24.357 101		1.00 14		A
13											
	MOTA	1607	СВ	LYS	220	21.666	24.380 101		1.00 12		A
	MOTA	1608	CG	LYS	220	22.360	25.077 100	.038	1.00 17	.07	A
	MOTA	1609	CD	LYS	220	23.833	25.326 100	.309	1.00 15	.93	A
	MOTA	1610	CE	LYS	220	24.512		.080	1.00 17		A
20											
20	MOTA	1611	NZ	LYS	220	25.991		.261	1.00 15		A
	MOTA	1612	С	LYS	220	19.718	23.360 99	.969	1.00 14	. 89	A
	MOTA	1613	0	LYS	220	19.497	23.722 98	. 809	1.00 15	.14	A.
	MOTA	1614	N	ARG	221	19.572	22.105 100	. 380	1.00 14	.35	A .
	MOTA	1615	CA	ARG	221	19.166		.492	1.00 15		A
25											
23	MOTA	1616	CB	ARG	221	19.185	19.714 100		1.00 14		A
	ATOM	1617	CG	ARG	221	19.467	18.488 99	. 455	1.00 18		A
	MOTA	1618	CD	ARG	221	19.485	17.273 100	. 365	1.00 20	.34	A
	MOTA	1619	NE	ARG	221 .	20.806	16.655 100	.446	1.00 21	.59	A
	MOTA	1620	CZ	ARG	221	21.148	15.748 101		1.00 21		A
30									1.00 19		
50	MOTA	1621		ARG	221	20.264	15.361 102				A
	ATOM	1622	NH2	ARG	221	22.367	15.218 101	.344	1.00 19	.97	Α
	MOTA	1623	С	ARG	221	17.761	21.290 98	. 932	1.00 15	.56	A
•	ATOM	1624	0	ARG	221	17.419	20.858 97	. 827	1.00 15	. 28	Α
	ATOM	1625	N	THR	222	16.945		.698	1.00 14		A
35											
22		. 1626	CA	THR	222	15.608		.253	1.00 13		A
•	MOTA	1627	CB	THR	222	14.781	22.963 100		1.00 16	.22	A
	ATOM	1628	OG1	THR	222	14.707	22.058 101	. 495	1.00 16	.19	A
	MOTA	1629	CG2	THR	222	13.367	23.252 99	.904	1.00 17	.44	A
	MOTA	1630	c	THR	222	15.679		.061	1.00 13		A
40											
40	MOTA	1631	0	THR	222	14.850		.156	1.00 12		A
	MOTA	1632	N	THR	223	16.667	24.175 98	.044	1.00 11	. 79	Α
	ATOM	1633	CA	THR	223	16.787	25.112 96	. 936	1.00 13	.70	A
	ATOM	1634	CB	THR	223	17.675	26.345 97	. 287	1.00 14	. 50	A
	ATOM	1635	0G1		223	19.058		.247	1.00 18		A
45											
40	MOTA	1636		THR	223	17.343		. 669	1.00 10		A
	MOTA	1637	С	THR	223	17.387	24.398 95	.729	1.00 15	.22	A
	ATOM	1638	0	THR	223	17.148	24.778 94	.580	\cdot 1.00 17	.54	A
	ATOM	1639	N	ALA	224	18.176	23.361 95	.986	1.00 14	.46	Α
	ATOM	1640	CA	ALA	224	18.773		.896	1.00 13		A
50									1.00 14		
50	MOTA	1641	CB	ALA	224	19.793		.432		-	A
	MOTA	1642	С	ALA	224	17.665		.171	1.00 13		A
	MOTA	1643	0	ALA	224	17.672	21,775 92	. 958	1.00 13	. 24	A
	MOTA	1644	N	ALA	225	16.710	21.346 94	. 932	1.00 13	. 91	A
	ATOM	1645	CA	ALA	225	15.598		.369	1.00 15		A
55	ATOM	1646	СВ	ALA	225	14.817		.498	1.00 15		A
55									1.00 13		
	MOTA	1647	C	ALA	225	14.640		.498			A
	MOTA	1648	0	ALA	225	14.070	20.908 92	.532	1.00 13	.24	A
	ATOM	1649	N	THR	226	14.449	22.694 93	. 822	1.00 15	.56	A
	MOTA	1650	CA	THR	226	13.555		.995	1.00 16	. 82	A
60	MOTA	1651	CB	THR	226	12.992		.747	1.00 17		A
OO.											
	MOTA	1652		THR	226	13.314		.015	1.00 21		A
	MOTA	1653	CG2	THR	226	13.557	24.822 95	.142	1.00 16		Α
	ATOM	1654	С	THR	226	14.300	23.943 91	.745	1.00 15	.61	A
	ATOM	1655	0	THR	226	13.685		.726	1.00 13		A
65	MOTA	1656	N	LEU	227	15.629		.828	1.00 14		Ä
55											
	MOTA	1657	CA	LEU	227	16.473		.716	1.00 14		A
	ATOM	1658	CB	LEU	227	17.751		.267	1.00 17		A
	ATOM	1659	CG	LEU	227	18.827	25.459 90	. 285	1.00 22	.76	A
	ATOM	1660		LEU	227	18.209		.160	1.00 21		A
70	ATOM	1661		LEU	227	19.873		.055	1.00 24		A
						16.808					
	ATOM	1662	C	LEU	227			.742	1.00 15		A
	ATOM	1663	Ο.	LEU	227	16.939		.540	1.00 16		A
	MOTA	1664	N	MET	228	16.924	22.000 90	.256	1.00 13	. 63	Α

		1.665				17 244	20 042	00 404		
	MOTA	1665	CA	MET	228	17.244	20.842	89.424	1.00 14.22	A
	ATOM ATOM	1666 1667	CB	MET MET	228 228	18.607 19.771	20.275 21.243	89.852 89.583	1.00 17.08 1.00 18.22	, A A
	ATOM	1668	CG SD	MET	228	21.340	20.816	90.414	1.00 19.64	Ä
5	ATOM	1669	CE	MET	228	21.189	21.761	91.964	1.00 16.95	Â
-	ATOM	1670	Č.	MET	228	16.148	19.768	89.504	1.00 13.11	A
	MOTA	1671	ō	MET	228	15.683	19.423	90.588	1.00 10.34	A
	ATOM	1672	N	ASN	229	15.748	19.243	88.348	1.00 12.86	A
	ATOM	1673	CA	ASN	229	14.676	18.246	88.259	1.00 13.74	Ä
10	ATOM	1674	CB	ASN	229	14.319	17.975	86.794	1.00 13.77	A
	MOTA	1675	CG	ASN	229	13.993	19.241	86.023	1.00 15.98	· A
	MOTA	1676	OD1		229	13.899	19.221	84.790	1.00 16.80	A
	MOTA	1677	ND2	ASN	. 229	13.814	20.352	86.740	1.00 15.44	A
	MOTA	1678	С	ASN	229	14.976	16.915	88.930	1.00 14.79	A
15	MOTA	1679	0	ASN	229	16.036	16.322	88.713	1.00 15.96	A
	MOTA	1680	N	ALA	230	14.022	16.444	89.728	1.00 12.65	. А
	ATOM	1681	CA	ALA	230	14.155	15.182	90.443	1.00 13.20	` A
	MOTA	1682	CB	ALA	230	13.971	14.010	89.476	1.00 11.65	A
20	MOTA	1683	C	ALA	230	15.514	15.099	91.114	1.00 12.14	A
20	MOTA	1684	0	ALA	230	16.187	14.071	91.056	1.00 11.89	A
	ATOM	1685	N	TYR	231	15.906	16.190	91.753	1.00 11.37	A
	MOTA	1686	CA	TYR	231	17.190	16.270	92.435	1.00 12.67	A
	MOTA	1687	CB	TYR	231	17.325	17.625	93.128	1.00 13.10	A
25	MOTA	1688	CG	TYR	231	18.685	17.843	93.720	1.00 13.58	A
25	MOTA	1689 1690		TYR	231	18.951	17.526	95.050 95.583	1.00 15.59 1.00 15.33	· A
	MOTA MOTA	1691	CE1	TYR TYR	231 231	20.235 19.728	17.687 18.325	92.934	1.00 14.58	· A A
	MOTA	1692		TYR	231	21.008	18.489	93.454	1.00 15.62	À
	ATOM	1693	cz	TYR	231	21.251	18.169	94.777	1.00 14.53	Ä
30	MOTA	1694	ОН	TYR	231	22.508	18.355	95.291	1.00 16.72	Ä
	MOTA	1695	C	TYR	231	17.431	15.162	93.458	1.00 12.52	A
	ATOM	1696	ō	TYR	231	18.470	14 500	93.436	1.00 12.31	A
	MOTA	1697	N	SER	232.	16.457	14.968	94.341	1.00 12.51	A
	MOTA	1698	CA	SER	232	16.543	13.978	95.406	1.00 11.76	A
35	ATOM	1699	CB	SER	232	15.325	14.091	96.331	1.00 10.64	A
	ATOM	1700	OG	SER	232	14.143	13.654	95.692	1.00 10.59	A
	MOTA	1701	С	SER	232	16.691	12.534	94.936	1.00 12.25	A
	MOTA	1702	0	SER	232	17.123	11.673	95.702	1.00 12.40	A
40	MOTA	1703	N	SER	233	16.332	12.244	93.695	1.00 11.36	À
40	MOTA	1704	CA	SER	233	16.485	10.876	93.241	1.00 12.78	A
	ATOM	1705	CB	SER	233	15.146	10.341	92.712	1.00 13.58	À
	MOTA	1706	OG	SER	233	. 14.735	11.011	91.547	1.00 17.87	A
	MOTA MOTA	1707 1708	C	SER SER	233 233	17.598 18.129	10.719 9.628	92.199	1.00 12.96 1.00 12.33	A A
45	ATOM	1709	N	ARG	234	17.984	11.817	91.552	1.00 12.33	Ä
43	ATOM	1710	CA	ARG	234	19.022	11.770	90.519	1.00 13.08	À
	ATOM	1711	CB	ARG	234	18.639	12.658	89.333	1.00 13.88	A
	ATOM	1712	CG	ARG	234	17.411	12.209	88.575	1.00 15.89	Ä
	MOTA	1713	CD	ARG	234	17.135	13.146	87.408	1.00 16.18	A
50	ATOM	1714	NE	ARG	234	15.961	12.713	86.672	1.00 20.62	A
	ATOM	1715	CZ	ARG	234	15.330	13.442	85.761	1.00 21.81	A
	MOTA	1716	NH1	ARG	234	15.764	14.662	85.459	1.00 21.30	A
	ATOM	· 1717	NH2	ARG	234	14.249	12.951	85.168	1.00 21.53	A
	MOTA	1718	C	ARG	234	20.409	12.182	90.972	1.00 11.75	A
55	MOTA	1719	0	ARG	234	21.374	12.011	90.230	1.00 11.05	A
	MOTA	1720	N	SER	235	20.510	12.744	92.170	1.00 9.69	A
	MOTA	1721	CA	SER	235	21.802	13.185	92.679	1.00 9.62	A
	ATOM	1722	CB	SER	235	21.656	14.525	93.409	1.00 9.37	A
60	MOTA	1723	OG	SER	235	20.858	14.410	94.575	1.00 9.00	A
UU	MOTA	1724	C	SER	235	22.445	12.171	93.617	1.00 9.66	A
	MOTA	1725	0	SER	235	21.768	11.317	94.190	1.00 12.40	A
	MOTA	1726	N	HIS	236	23.762	12.287	93.758	1.00 8.64 1.00 5.39	A
	MOTA MOTA	1727 1728	CA CB	HIS	236 236	24.573 25.795	11.436 10.898	94.627 93.878	1.00 5.39 1.00 6.60	A A
65	ATOM	1729	CG	HIS	236	25.474	10.085	92.666	1.00 6.36	A
J.J	ATOM	1730		HIS	236	25.516	10.003	91.350	1.00 6.40	A
	MOTA	1731		HIS	236	25.109	8.758	92.732	1.00 6.26	A
	MOTA	1732		HIS	236	24.945	8.287	91.509	1.00 4.95	Ä
	MOTA	1733		HIS	236	25.186	9.261	90.652	1.00 5.93	Ä
70	MOTA	1734	C	HIS	236	25.092	12.348	95.732	1.00 6.58	A
	MOTA	1735	0	HIS	236	25.676	13.396	95.446	1.00 5.89	A
	ATOM	1736	N	SER	237	24.902	11.972	96.990	1.00 7.32	A
	MOTA	1737	CA	SER	237	25.409	12.816	98.063	1.00 7.91	A

•	MOTA	1738	CB	SER	237	24.28	7 13:204	99.022	1.00 8.40	A
	MOTA	1739	OG	SER	237	23.89	5 12.093	99.805	1.00 12.48	A
	MOTA	1740	C	SER	237	26.50		98.830	1.00 7.51	A
	MOTA	1741	ō	SER	237	26.36		99.179	1.00 10.56	A
5	MOTA	1742	N	VAL	238	27.59		99.092	1.00 7.01	A
-	MOTA	1743	CA	VAL	238	28.71		99.822	1.00 7.37	A
	MOTA			VAL	238	30.03		98.998	1.00 8.80	Ä
		1744	CB			31.14				
	MOTA	1745		VAL	238		-	99.741		A
10	MOTA	1746		VAL	238	29.83		97.603	1.00 5.26	A
10	MOTA	1747	С	VAL	238	28.93		101.107	1.00 8.29	A
	MOTA	1748	·O	VAL	238	29.44		101.057	1.00 8.87	A
	MOTA	1749	N	PHE	239	28.54	9 12.454	102.247	1.00 7.65	A
	ATOM	1750	CA	PHE	239	28.75	6 13.114	103.531	1.00 7.41	A
_	ATOM	1751	CB	PHE	239	27.55	7 12.895	104.454	1.00 7.34	A
15	MOTA	1752	CG	PHE	239	27.61	5 13.694	105.726	1.00 6.91	A
	ATOM	1753		PHE	239	28.50	8 13.355	106.744	1.00 7.70	A
	MOTA	1754		PHE	239	26.77		105.906	1.00 6.68	A
	ATOM	1755		PHE	239	28.56		107.931	1.00 7.54	A
	MOTA	1756		PHE	239	26.82		107.086	1.00 8.52	A
20	ATOM	1757	CZ	PHE	239	27.72		108.101	1.00 7.57	A
20		1758	č	PHE	239	30.01		104.169	1.00 10.17	A
	MOTA			PHE	239	30.06			1.00 10.17	
	MOTA	1759	0					104.486		A .
	MOTA	1760	N	SER	240	31.03		104.350	1.00 9.89	A
25	MOTA	1761	CA	SER	240	32.28		104.926	1.00 11.46	A
25	MOTA	1762	CB	SER	240	33.44		103.966	1.00 10.05	A
	MOTA	1763	OG	SER	240	33.18		102.681	1.00 14.59	A
	MOTA	1764	С	SER	240	32.59		106.285	1.00 12.92	A
	MOTA	1765	0	SER	240	32.40		106.509	1.00 12.61	A
20	MOTA	1766	N	VAL	241	33.07		107.193	1.00 12.52	A
30	MOTA	1767	CA	VAL	241	33.46		108.511	1.00 13.59	A
	MOTA	1768	CB	VAL	241	32.55		109.613	1.00 14.83	A
	MOTA	1769	CG1	VAL	241	32.52	6 10.991	109.492	1.00 17.21	A
	MOTA	1770	CG2	VAL	241	33.05	4 12.922	110.993	1.00 13.88	A
	MOTA	1771	С	VAL	241	34.93	1 12.718	108.731	1.00 13.59	A
35	MOTA	·1772	0	VAL	241	35.30	5 11.548	108.607	1.00 10.71	A
	MOTA	1773	N	THR	242	35.75	9 13.715	109.024	1.00 14.44	A
	MOTA	1774	CA	THR	242	37.17		109.264	1.00 15.80	A
	MOTA	1775	CB	THR	242	38.05		108.409	1.00 16.64	A
	MOTA	1776	OG1		242	37.71		107.025	1.00 19.41	A
40	ATOM	1777	CG2	THR	242	39.53		108.618	1.00 11.48	A
	ATOM	1778	c	THR	242	37.47		110.734	1.00 17.79	Ä
	ATOM	1779	ŏ	THR	242	37.05		111.322	1.00 19.50	A
	MOTA	1780	N	ILE	243	38.22		111.326	1.00 18.66	A
	ATOM	1781	CA	ILE	243	38.56		112.730	1.00 20.82	Ä
45	ATOM	1782	CB	ILE	243	37.97		113.500	1.00 20.34	A
73	MOTA	1783	-	ILE	243	38.08		114.993	1.00 20.79	Ä
				ILE	243	36.50		113.114	1.00 21.41	Ä
	MOTA	1784								
	MOTA	1785		ILE	243	35.90		113.632	1.00 20.85	A
50	MOTA	1786	C	ILE	243	40.07		112.958	1.00 23.56	A
20	MOTA	1787	0	ILE	243	40.78		112.664	1.00 23.06	A
	MOTA	1788	N	HIS	244	40.57		113.458	1.00 25.26	A
	ATOM	1789	CA	HIS	244	. 41.99		113.765	1.00 27.63	. A
	MOTA	1790	CB	HIS	244	42.50		113.485	1.00 28.72	A
	ATOM	1791	CG	HIS	244	42.97		112.079	1.00 32.69	A
55	MOTA	1792		HIS	244	44.21		111.544	1.00 33.88	A
	MOTA	1793	ND1	HIS	244	42.11		111.038	1.00 34.05	A
	MOTA	1794	CE1	HIS	244	42.80		109.924	1.00 33.87	A
	MOTA	1795	NE2	HIS	244	44.08		110.203	1.00 35.45	A -
	ATOM	1796	С	HIS	244	42.10	8 13.878	115.254	1.00 29.05	· A
60	MOTA	1797	0	HIS	244	41.54	14.599	116.084	1.00 28.16	A
	ATOM	1798	N	MET	245	42.82	7 12.813	115.592	1.00 29.99	A
	MOTA	1799	CA	MET	245	42.96		116.988	1.00 32.41	A
	MOTA	1800	CB	MET	245	42.33		117.210	1.00 30.98	A
	ATOM	1801	CG	MET	245	40.88		116.795	1.00 29.47	A
65	ATOM	1802	SD	MET	245	40.39		116.608	1.00 28.28	Ä
55	MOTA	1803	CE	MET	245	41.01		114.953	1.00 26.37	A
	ATOM	1804	C	MET	245	44.39		117.520	1.00 28.37	Â
	MOTA	1805	0	MET	245	45.33		116.831	1.00 33.45	, A
	ATOM	1806		LYS	245	44.53		118.765	1.00 36.79	. A
70	ATOM		N	LYS	246	45.81		119.456	1.00 36.79	
, 0		1807 1808	CA		246			119.456	1.00 41.41	A
	ATOM		CB	LYS		46.34				A
	ATOM	1809	CG	LYS	246	47.76		120.187	1.00 48.98	A
	MOTA	1810	CD	LYS	246	48.36	,U 13.0/8	120.048	1.00 52.77	A

	MOTA	1811	CE	LYS	246	49.830	15.693	120.448	1.00 55.09	A
	MOTA	1812	NZ	LYS	246	50.445	17.035		1.00 56.33	A
	ATOM	1813	c	LYS	246	45.496	12.179		1.00 42.14	A
	ATOM	1814	ō	LYS	246	45.157	12.860		1.00 42.94	A
5	ATOM	1815	N	GLU	247	45.586	10.859		1.00 42.88	A
,	MOTA	1816	CA	GLU	247	45.286	10.090		1.00 45.27	Ä
	ATOM	1817	СВ	GLU	247	44.896		121.623	1.00 45.22	A
		1818	CG	GLU	247	44.301		122.726	1.00 45.70	À
	ATOM	1819		GLU	247		6.396		1.00 47.91	À
10	MOTA		CD						1.00 48.39	A
10	MOTA	1820		GLU	247	43.507		121.186	1.00 47.23	
	MOTA	1821	OE2	GLU	247	44.462		123.032		
	MOTA	1822	C	GLU	247	46.463	10.040		1.00 46.56	A
	ATOM	1823	0	GLU	247	47.625	10.055		1.00 46.38	A
15	MOTA	1824	N	THR	248	46.144		124.281	1.00 47.43	A
15	MOTA	1825	CA	THR	248	47.155		125.320	1.00 49.03	A
	MOTA	1826	CB	THR	248	47.340	11.259		1.00 49.86	A
	MOTA	1827		THR	248	47.733	12.245		1.00 50.38	A
	MOTA	1828		THR	248	48.416	11.162		1.00 49.64	A
20	MOTA	1829	С	THR	248	46.679		126.309	1.00 49.49	A
20	MOTA	1830	0	THR	248	45.810		127.148	1.00 49.04	A
	MOTA	1831	N	THR	249	47.244		126.177	1.00 50.47	A
	ATOM	1832	CA	THR	249	46.892		127.025	1.00 51.50	A
	MOTA	1833	CB	THR	249	47.684		126.621	1.00 51.30	A
~~	MOTA	1834	OG1	THR	249	49.072	5.435	126.933	1.00 50.45	A
25	MOTA	1835	CG2	THR	249	47.539	4.994	125.127	1.00 50.34	· A
	MOTA	1836	С	THR	249	47.157	6.813	128.493	1.00 52.76	. А
	MOTA	1837	0	THR	249	47.801	7.811	128.819	1.00 52.66	A
	MOTA	1838	N	ILE	250	46.663	5.948	129.375	1.00 53.97	A
	MOTA	1839	CA	ILE	250	46.842	6.136	130.812	1.00 55.19	A
30	MOTA	1840	CB	ILE	250	46.042	5.078	131.624	1.00 55.38	A
	MOTA	1841	CG2	ILE	250	44.596	5.061	131.147	1.00 55.55	A
	MOTA	1842	CG1	ILE	250	46.656	3.683	131.466	1.00 55.59	A
	ATOM	1843	CD1	ILE	250	46.516	3.078	130.073	1.00 56.12	A
	MOTA	1844	С	ILE	250	48.313	6.097	131.239	1.00 55.82	A
35	MOTA	1845	0	ILE	250	48.634	6.316	132.408	1.00 55.54	A
	MOTA	1846	N	ASP	251	49.198	5.833	130.281	1.00 56.61	A
	ATOM	1847	CA	ASP	251	50.633		130.543	1.00 57.44	A
	ATOM	1848	СВ	ASP	251	51.285		129.679	1.00 57.92	A
	MOTA	1849	CG	ASP	251	50.757		129.979	1.00 58.92	A
40	ATOM	1850		ASP	251	50.894		129.098	1.00 59.53	Ä
	ATOM	1851		ASP	251	50.217		131.089	1.00 57.67	A
	ATOM	1852	C	ASP	251	51.271		130.222	1.00 57.89	A
	ATOM	1853	ŏ	ASP	251	51.858		131.090	1.00 59.32	A
	ATOM	1854	N	GLY	252	51.141		128.967	1.00 57.36	A
45	ATOM	1855	CA	GLY	252	51.707		128.526	1.00 57.52	A
	ATOM	1856	c	GLY	252	52.089		127.060	1.00 57.92	A
	MOTA	1857	ō	GLY	252	52.814		126.545	1.00 58.43	A
	ATOM	1858	N	GLU	253	51.602		126.392	1.00 57.56	A
	MOTA	1859	CA	GLU	253	51.869		124.974	1.00 57.81	A
50	MOTA	1860	CB	GLU	253	51.552		124.598	1.00 59.90	A
50	MOTA	1861	CG	GLU	253	52.084		125.573	1.00 62.49	A
	MOTA	1862	CD	GLU	253	51.543		125.294	1.00 63.65	A
	ATOM	1863		GLU	253	51.693		124.146	1.00 65.45	A
	ATOM	1864		GLU	253	50.970		126.219	1.00 63.15	Ä
55	ATOM	1865	C	GLU	253	50.959		124.179	1.00 56.36	A
33	ATOM	1866	ŏ	GLU	253	49.818		124.572	1.00 56.13	Ä
			N	GLU	254	51.451		123.067	1.00 54.64	Ä
	ATOM ATOM	1867 1868	CA	GLU	254	50.626	0.300	122.256	1.00 53.82	Ä
		1869			254	51.269		122.151	1.00 54.89	Ä
60	MOTA		CB	GLU				121.354	1.00 56.86	
00	ATOM	1870	CG	GLU	254	52.568		119.939	1.00 58.42	A
	ATOM	1871	CD	GLU	254	52.363				A
	MOTA	1872		GLU	254	51.856		119.800	1.00 58.67 1.00 57.93	A
	MOTA	1873		GLU	254	52.713		118.968		A
65	ATOM	1874	C	GLU	254	50.397		120.876	1.00 52.35 1.00 52.94	· A
UJ	ATOM	1875	0	GLU	254	51.340		120.124		A
	ATOM	1876	N	LEU	255	49.135		120.560	1.00 50.68	A
	ATOM	1877	CA	LEU	255	48.772		119.268	1.00 48.63	A
	ATOM	1878	CB	LEU	255	47.828		119.439	1.00 49.85	A
70	ATOM	1879	CG	LEU	255	48.236		120.231	1.00 52.23	A
70	MOTA	1880		LEU	255	49.595		119.752	1.00 53.67	A
	ATOM	1881		LEU	255	48.278		121.720	1.00 53.72	Ä
	ATOM	1882	C	LEU	255	48.069		118.413	1.00 46.05	A
	ATOM	1883	0	LEU	255	46.978	9.832	118.755	1.00 45.38	A

										_
•	MOTA	1884	N	VAL	256	48.695		117.310	1.00 43.74	A
	MOTA	1885	CA	VAL	256	48.081		116.409	1.00 41.19	A
	MOTA	1886	CB	VAL	256	49.084		115.943	1.00 40.17	A
_	MOTA	1887		VAL	256	48.442		114.897	1.00 38.91	A
5	MOTA	1888	CG2	VAL	256	49.543		117.132	1.00 40.08	A
	ATOM	1889	С	VAL	256	47.533		115.200	1.00 39.59	Ą
	MOTA	1890	0	VAL	256	48.276	9.619	114.291	1.00 39.95	A
	MOTA	1891	N	LYS	257	46.221	9.780	115.212	1.00 36.47	Α
	ATOM	1892	CA	LYS	257	45.534	9.056	114.150	1.00 32.43	A
10	ATOM	1893	CB	LYS	257	44.733	7.902	114.756	1.00 31.46	A
	MOTA	1894	CG	LYS	257	45.525		115.710	1.00 31.17	A
	MOTA	1895	CD	LYS	257	44.613		116.573	1.00 30.49	A
	MOTA	1896	CE	LYS	257	43.767		117.486	1.00 31.11	A
•	MOTA	1897	NZ.	LYS	257	42.941		118.411	1.00 32.10	Ä
15	MOTA	1898	C	LYS	257	44.585		113.384	1.00 30.18	Ä
1.5	MOTA	1899	ŏ	LYS	257	44.067		113.928	1.00 28.57	A
•		1900	N	ILE	258	44.361		112.120	1.00 28.11	A
	MOTA				258	43.451		111.263	1.00 26.14	Ä
	ATOM	1901	CA	ILE				110.209	1.00 26.23	A
20	MOTA	1902	CB	ILE	258	44.223				
20	ATOM	1903	CG2	ILE	258	43.265		109.205	1.00 26.22	A
	MOTA	1904	CG1	ILE	258	45.027		110.904	1.00 27.27	A
	MOTA	1905		ILE	258	45.828		109.943	1.00 29.18	Α.
	MOTA	1906	С	ILE	258	42.493		110.573	1.00 24.09	A
25	MOTA	1907	0	ILE	258	42.912		109.772	1.00 24.80	Ά
25	MOTA	1908	N	GLY	259	41.208		110.899	1.00 20.82	A
	MOTA	1909	CA	GLY	259	40.221		110.300	1.00 17.04	A
	MOTA	1910	С	GLY	259	39,214	9.376	109.447	1.00 15.18	A
	MOTA	1911	0	GLY	259	38.843	10.502	109.765	1.00 14.10	A
	MOTA	1912	N	LYS	260	38.782	8.764	108.349	1.00 13.62	A
30	MOTA	1913	CA	LYS	260	37.803	9.399	107.487	1.00 13.15	A
	ATOM	1914	СВ	LYS	260	38.480	9.983	106.247	1.00 13.95	A
	MOTA	1915	CG	LYS	260	37.557	10.866	105.414	1.00 14.12	A
	MOTA	1916	CD	LYS	260	38.254	11.500	104.220	1.00 14.32	A
	MOTA	1917	CE	LYS	260	37.256		103.410	1.00 16.28	A
35	ATOM	1918	NZ	LYS	260	37.881		102.307	1.00 14.26	A
	MOTA	1919	C	LYS	260	36.687		107.080	1.00 13.76	A
	MOTA	1920	ō.	LYS	260	36.939		106.612	1.00 14.46	A
	MOTA	1921	N	LEU	261			107.277	1.00 11.00	A
	MOTA	1922	CA	LEU	261	34.281		106.954	1.00 9.03	Ä
40	MOTA	1923	CB	LEU	261	33.461		108.217	1.00 6.67	Ä
70		1924	CG	LEU	261	32.123		108.093	1.00 3.68	Ä
	MOTA			LEU	261	32.319		100.093	1.00 2.23	Ä
	MOTA	1925						107.314	1.00 2.23	A
	MOTA	1926		LEU	261	31.499		105.905		
45	MOTA	1927	C	LEU	261	33.416			1.00 10.81	A
43	MOTA	1928	0	LEU	261	32.978		106.113	1.00 9.03	A
	MOTA	1929	N	ASN	262	33.180		104.786	1.00 8.62	A
	MOTA	1930	CA	ASN	262	32.360		103.702	1.00 9.89	A
	MOTA	1931	CB	ASN	262	33.042		102.348	1.00 10.45	A
50	MOTA	1932	CG.	ASN	262	34.436		102.294	1.00 14.30	A
50	MOTA	1933		ASN	262	35.420		102.136	1.00 16.96	A
	MOTA	1934		ASN	262	34.535		102.432	1.00 9.79	A
	MOTA	1935	C	ASN	262	31.003		103.721	1.00 9.32	. А
	MOTA	1936	0	ASN	262	30.940		103.638	1.00 10.83	A
	ATOM	1937	N	LEU	263	29.923		103.839	1.00 8.87	A
55	MOTA	1938	CA	LEU	263	28.572	8.108	103.874	1.00 8.66	A
	MOTA	1939	CB	LEU	263	27.832	8.607	105.108	1.00 6.12	A
	ATOM	1940	CG	LEU	263	28.620		106.375	1.00 8.11	A
	MOTA	1941	CD1	LEU	263	27.981	8.906	107.599	1.00 8.26	Α.
	MOTA	1942	CD2	LEU	263	28.679		106.520	1.00 5.47	A
60	ATOM	1943	С	LEU	263	27.878		102.595	1.00 10.21	A
	ATOM	1944	Õ	LEU	263	27.488		102.441	1.00 12.04	. A
	ATOM	1945	N	VAL	264	27.716		101.682	1.00 9.38	A
	ATOM	1946	CA	VAL	264	27.161		100.378	1.00 9.77	A
	ATOM	1947	CB	VAL	264	28.089	7.329	99.291	1.00 10.33	Ä
65	ATOM	1948		VAL	264	27.734	7.907	97.928	1.00 8.01	Ä
			CG2	VAL	264	29.522	7.637	99.672	1.00 8.80	Â
	ATOM	1949						100.104		
	MOTA	1950	C	VAL	264	25.765			1.00 10.32	A
	MOTA	1951	0	VAL	264	25.465		100.226	1.00 12.03	A
70	ATOM	1952	N	ASP	265	24.925	8.355	99.714	1.00 9.00	A
70	ATOM	1953	CA	ASP	265	23.534	8.116	99.368	1.00 6.24	A
	MOTA	1954	CB	ASP	265	22.650	9.211	99.985	1.00 5.48	A
	MOTA	1955	CG.	ASP	265	21.171	8.994	99.713	1.00 7.76	A
	MOTA	1956	OD1	ASP	265	20.851	8.232	98.782	1.00 5.27	A

										_
	MOTA	1957	OD2		265	20.328		100.421	1.00 9.82	A
	MOTA	1958	С	ASP	265	23.497	8.203	97.838	1.00 4.32	A
	ATOM	1959	0	ASP	265	23.410	9.289	97.270	1.00 4.24	A
	MOTA	1960	N	LEU	266	23.575	7.060	97.172	1.00 4.44	A
5	MOTA	1961	CA	LEU	266	. 23.569	7.024	95.710	1.00 5.61	A
	MOTA	1962	CB	LEU	266	23.941	5.616	95.222	1.00 1.02	A
	MOTA	1963	CG	LEU	266	25.345	5.124	95.622	1.00 5.57	A
	MOTA	1964		LEU	266	25.561	3.649	95.242	1.00 1.02	A
	ATOM	1965		LEU	266	26.379	6.020	94.942	1.00 4.62	A
10	ATOM	1966	c	LEU	266	22.252	7.451	95.065	1.00 7.56	A
10	MOTA	1967	ŏ	LEU	266	21.190	7.438	95.694	1.00 9.23	' A
	ATOM	1968	N	ALA	267	22.336	7.845	93.801	1.00 7.43	A
				ALA	267	21.156	8.220	93.047	1.00 6.36	Ä
	ATOM	1969	CA					91.687		Ä
15	ATOM	1970	CB	ALA	267	21.572	8.756			
13	ATOM	1971	C	ALA	267	20.324	6.945	92.877	1.00 6.99	A
	MOTA	1972	0	ALA	267	20.844	5.840	93.020	1.00 5.27	A
	MOTA	1973	N	GLY	268	19.042	7.105	92.571	1.00 9.81	A
	MOTA	1974	CA	GLY	268	18.170	5.961	92.378	1.00 12.51	A
20	MOTA	1975	С	GLY	268	18.633	5.079	91.233	1.00 15.67	A
20	ATOM	1976	0	GLY	268	18.859	5.555	90.113	1.00 17.12	A
	MOTA	1977	N	SER	269	18.755	3.786	91.516	1.00 15.31	A
	MOTA '	1978	CA	SER	269	19.220	2.802	90.543	1.00 18.23	A
	MOTA	1979	CB	SER	269	19.677	1.554	91.293	1.00 17.50	A
	ATOM	1980	OG	SER	269	18.596	1.027	92.043	1.00 12.64	Α
25	MOTA	1981	С	SER	269	18.195	2.383	89.484	1.00 20.29	Α
	ATOM	1982	0	SER	269	18.497	1.549	88.627	1.00 19.97	· A
	ATOM	1983	N	GLU	270	16.994	2.950	89.537	1.00 22.91	A
	ATOM	1984	CA	GLU	270	15.949	2.576	88.587	1.00 26.68	A
	ATOM	1985	CB	GLU	270	14.563	2.958	89.136	1.00 24.65	Α
30	ATOM	1986	CG	GLU	270	14.251	4.460	89.210	1.00 22.35	A
	MOTA	1987	CD	GLU	270	14.960	5.185	90.349	1.00 21.47	A
	ATOM	1988		GLU	270	15.545	4.524	91.234	1.00 18.55	A
	ATOM	1989		GLU	270 · ·	14.922	6.433	90.354	1.00 22.04	A
	ATOM	1990	C	GLU	270	16.117	3.139	87.177	1.00 31.14	A
35	ATOM	1991	ō	GLU	270	16.608	4.256	86.981	1.00 30.32	A
55	MOTA	1992	N	ASN	271	15.717	2.336	86.194	1.00 36.67	Ä
	ATOM	1993	CA	ASN	271	15.799	2.730	84.793	1.00 41.70	A
				ASN	271	16.856	1.900	84.059	1.00 45.31	Ä
	MOTA	1994	CB				2.409	82.649	1.00 49.20	Ä
40	ATOM	1995	CG	ASN	271	17.121			1.00 50.16	
40	MOTA	1996		ASN	271	17.661	3.504	82.460		A
	ATOM	1997	ND2	ASN	271	16.733	1.618	81.650	1.00 50.41	A
	MOTA	1998	C	ASN	271	14.440	2.537	84.120	1.00 42.80	A
	ATOM	1999	0	ASN	271	13.799	1.494	84.276	1.00 44.21	À
45	MOTA	2000	N	ASN	287	17.192	11.408	81.710	1.00 47.26	A
45·	MOTA	2001	CA	ASN	287	18.348	11.168	80.854	1.00 46.49	A
	ATOM	2002	CB	ASN	287	19.078	12.487	80.582	1.00 48.42	A
	MOTA	2003	CG	ASN	287	18.323	13.385	79.614	1.00 51.20	A
	ATOM	2004	OD1	ASN	287	18.724	14.526	79.368	1.00 51.62	A
	MOTA	2005	ND2	ASN	287	17.230	12.870	79.053	1.00 50.69	A
50	MOTA	2006	С	ASN	287	19.324	10.139	81.437	1.00 45.61	A
	MOTA	2007	0	ASN	287	18.912	9.131	82.021	1.00 45.57	A
	MOTA	2008	N	ILE	288	20.619	10.400	81.285	1.00 42.07	A
	MOTA	2009	CA	ILE	288	21.634	9.471	81.771	1.00 37.70	A
	MOTA	2010	CB	ILE	288	22.657	9.156	80.646	1.00 39.37	A
55	MOTA	2011	CG2	ILE	288	21.964	8.416	79.511	1.00 38.36	A
	ATOM	2012	CG1	ILE	288	23.269	10.450	80.095	1.00 40.59	A
	MOTA	2013		ILE	288	24.498	10.959	80.863	1.00 42.56	A
	MOTA	2014	C	ILE	288	22.385	9.924	83.019	1.00 33.61	A
	ATOM	2015	Õ	ILE	288	22.668	11.113	83.194	1.00 34.30	A
60	MOTA	2016	N	ASN	289	22.682	8.970	83.897	1.00 26.00	A
00	ATOM	2017	CA	ASN	289	23.431	9.267	85.107	1.00 19.08	A
	ATOM	2017	CB	ASN	289	22.810	8.599	86.334	1.00 17.79	Ä
	ATOM	2019	CG	ASN	289	23.253	9.253	87.645	1.00 17.75	Ä
		2019		ASN	289	22.461	9.928	88.299	1.00 18.10	Ä
65	MOTA				289		9.065	88.023	1.00 13.15	A
UJ	MOTA	2021		ASN		24.516		84.861		
	MOTA	2022	C	ASN	289	24.808	8.679		1.00 15.55	A
	MOTA	2023	0	ASN	289	25.033	7.493	85.072	1.00 12.50	A
	MOTA	2024	N	GLN	290	25.727	9.515	84.398	1.00 13.86	A
70	MOTA	2025	CA	GLN	290	27.079	9.070	84.088	1.00 12.24	A
70	MOTA	2026	CB	GLN	290	27.896	10.253	83.560	1.00 11.18	A
	MOTA	2027	CG	GLN	290	29.284	9.913	83.068	1.00 10.23	A
	MOTA	2028	CD	GLN	290	29.297	8.795	82.036	1.00 11.80	A
	MOTA	2029	OE1	GLN	290	28.336	8.609	81.273	1.00 12.41	A

	ATOM	2030	NE2	GLN	290	30.399	8:059	81.990	1.00 10.69	A
		2031	C	GLN	290	27.778	8.414	85.276	1.00 11.63	A
	MOTA									
	ATOM	2032	0	GLN	290	28.394	7.359	85.130	1.00 12.20	A
	MOTA	2033	N	SER	291	27.662	9.023	86.452	1.00 10.76	A
5	MOTA	2034	CA	SER	291	28.304	8.485	87.650	1.00 11.04	A
-	ATOM	2035	CB	SER	291	28.163	9.450	88.830	1.00 10.12	A
•	ATOM	2036	OG	SER	291	29.068	10.536	88.711	1.00 11.06	A
	ATOM	2037	С	SER	291	27.753	7.131	88.043	1.00 11.79	A
	ATOM	2038	0	SER	291	28.512	6.241	88.420	1.00 14.45	A
10	ATOM	2039	N	LEU	292	26.437	6.971	87.959	1.00 11.86	A
10										
	MOTA	2040	·CA	LEU	292	25.805	5.709	88.312	1.00 10.53	A
	MOTA	2041	CB	LEU	292	24.278	5.875	88.329	1.00 10.11	A
	MOTA	2042	CG	LEU	292	23.467	4.734	88.952	1.00 11.58	A
	ATOM	2043	CD1	LEU	292	23.811	4.605	90.427	1.00 9.76	A
15	MOTA	2044		LEU	292	21.974	5.007	88.791	1.00 11.92	A
15					292			87.289	1.00 10.87	
	MOTA	2045	C	LEU		26.216	4.653			A
	ATOM	2046	0	LEU	292	26.559	3.525	87.634	1.00 12.05	A
	ATOM	2047	N	LEU	293	26.196	5.043	86.022	1.00 11.04	A
	MOTA	2048	CA	LEU	293	26.566	4.165	84.929	1.00 11.19	A
20	ATOM	2049	CB	LEU	293	26.382	4.922	83.608	1.00 11.77	A
20										
	MOTA	2050	CG	LEU	293	25.394	4.442	82.532	1.00 15.36	Ā
	MOTA	2051	CD1	LEU	293	24.197	3.755	83.162	1.00 13.37	A,
	MOTA	2052	CD2	LEU	293	24.948	5.638	81.690	1.00 11.70	A
	ATOM	2053	С	LEU	293	28.026	3.714	85.094	1.00 13.10	·A
25	MOTA	2054	ō	LEU	293	28.355	2.535	84.918	1.00 13.28	A
25							4.660	85.437		
	MOTA	2055	N	THR	294	28.896			1.00 11.21	A
	MOTA	2056	CA	THR	294	30.313	4.372	85.613	1.00 10.86	A
	MOTA	2057	ÇВ	THR	294	31.119	5.690	85.778	1.00 12.02	A
	ATOM	2058	0G1	THR	294	30.934	6.497	84.611	1.00 11.95	A
30	ATOM	2059		THR	294	32.605	5.409	85.947	1.00 8.75	A
50				THR	294	30.571	3.459	86.809	1.00 11.13	A
	MOTA	2060	C							
	MOTA	2061	0	THR	294	31.416	2.563	86.735	1.00 10.49	A
	MOTA	2062	N	LEU	295	29.843	3.686	87.906	1.00 11.70	A
	ATOM	2063	CA	LEU	295	29.983	2.870	89.117	1.00 11.27	A
35	ATOM	2064	CB	LEU	295	29.033	3.348	90.224	1.00 10.76	A
					295	28.993	2.535	91.529	1.00 10.99	A
•	ATOM	2065	CG	LEU						
	MOTA	2066		LEU	295	30.352	2.540	92.214	1.00 12.41	A
	ATOM	2067	CD2	LEU	295	27.950	3.126	92.458	1.00 10.86	A
	ATOM	2068	С	LEU	295	29.683	1.424	88.788	1.00 10.80	A
40	ATOM	2069	0	LEU	295	30.365	0.521	89.252	1.00 12.59	A
	MOTA	2070	N	GLY		28.652	1.205	87.986	1.00 11.95	A
	MOTA	2071	CA	GLY	296	28.311	-0.153	87.607	1.00 12.43	A
	MOTA	2072	С	GLY	296	29.444	-0.772	86.810	1.00 13.06	A
	ATOM	2073	0	GLY	296	29.796	-1.938	87.007	1.00 15.18	A
45	ATOM	2074	N	ARG	297	30.021	0.014	85.906	1.00 11.06	A
	ATOM	2075	CA	ARG	297	31.121	-0.458	85.086	1.00 9.97	A
				ARG			0.517	83.943	1.00 9.77	A
	MOTA	2076	CB		297	31.369				
	MOTA	2077	CG	ARG	297	30.264	0.487	82.909	1.00 10.57	A
	ATOM	2078	CD.	ARG	297	30.173	1.789	82.136	1.00 8.79	Α
50	MOTA	·2079	NE	ARG	297	29.014	1.776	81.259	1.00 10.33	A
	ATOM	2080	CZ	ARG	297	28.492	2.853	80.685	1.00 9.93	A
	ATOM	2081	NH1		297	29.033	4.044	80.892	1.00 10.65	A
				ARG		27.412	2.740	79.920	1.00 7.47	A
	MOTA	2082			297					
c e	ATOM	2083	С	ARG	297	32.395	-0.675	85.889	1.00 9.24	A
55	ATOM	2084	0	ARG	297	33.154	-1.597	85.594	1.00 10.04	A
	MOTA	2085	N	VAL	298	32.632	0.164	86.897	1.00 6.73	A
	ATOM	2086	CA	VAL	298	33.823	0.009	87.734	1.00 7.78	A
	ATOM	2087		VAL	298	33.988	1.196	88.719	1.00 7.07	A.
			CB							
6 0	MOTA	2088		VAL	298	35.026	0.865	89.773	1.00 2.16	A
60	MOTA	2089	CG2	VAL	298	34.408	2.449	87.957	1.00 4.22	A
	MOTA	2090	С	VAL	298	33.775	-1.315	88.517	1.00 9.86	A
	MOTA	2091	ŏ	VAL	298	34.761	-2.057	88.556	1.00 11.69	A
	MOTA	2092	N	ILE	299	32.625	-1.616	89.120	1.00 10.47	A
									1.00 10.02	
65	MOTA	2093	CA	ILE	299	32.437	-2.858	89.879		A
65	MOTA	2094	CB	ILE	299	31.004	-2.910	90.488	1.00 10.33	A
	ATOM	2095	CG2	ILE	299	30.710	-4.280	91.095	1.00 9.07	A
	ATOM	2096		ILÈ	299	30.869	-1.821	91.558	1.00 10.35	A
	ATOM	2097		ILE	299	29.445	-1.587	92.019	1.00 13.51	A
					299		-4.070	88.972	1.00 11.19	Ā
70	MOTA	2098	C	ILE		32.659				
70	MOTA	2099	0	ILE	299	33.341	-5.019	89.348	1.00 9.09	, А
	ATOM	2100	N	THR	300	32.084	-4.031	87.771	1.00 14.08	A
	ATOM	2101	CA.	THR	300	32.227	-5.125	86.808	1.00 13.98	A
	ATOM	2102	CB	THR	300	31.470	-4.813	85.506	1.00 13.76	A
					-					

	MOTA	2103	OG1	THE	. 300	30.062	-4.803	85.770	1.00 14.55	A
									1.00 10.43	Α
	MOTA	2104	CG2		300	31.783	-5.848	84.436		
	MOTA	2105	C,	THR	300	33.699	-5.394	86.472	1.00 16.17	A
		2106	ŏ	THR	300	34.151	-6.536	86.533	1.00 16.23	A
_	MOTA									
5	MOTA	2107	N	ALA	301	34.442	-4.345	86.120	1.00 15.12	A
	MOTA	2108	CA'	ALA	301	35.850	~4.502	85.791	1.00 14.70	A
								85.362	1.00 13.94	
	MOTA	2109	СВ	ALA	301	36.449	-3.157			A
	MOTA	2110	C	ALA	301	36.622	-5.068	86.985	1.00 14.94	A
	ATOM	2111	Ó	ALA	301	37.512	-5.893	86.819	1.00 15.20	A
10										
10	MOTA	2112	N	LEU	302	36.282	-4.620	88.188	1.00 16.14	A
	MOTA	2113	CA	LEU	302	36.951	-5.101	89.392	1.00 19.53	· А
			СВ	LEU	302	36.585	-4.222	90.594	1.00 19.74	A
	MOTA	2114								
	MOTA	2115	CG	LEU	302	37.221	-2.830	90.688	1.00 17.91	A
	MOTA	2116	CD1	LEU	302	36.558	-2.045	91.802	1.00 17.40	A
15							-2.963	90.948	1.00 15.50	A
1)	MOTA	2117	CD2		302	38.717				
	MOTA	2118	С	LEU	302	36.643	-6.564	89.717	1.00 21.83	A
	MOTA	2119	0	LEU	302	37.533	-7.302	90.127	1.00 23.13	Α
	MOTA	2120	N	VAL	303	35.398	-6.993	89.535	1.00 24.49	A
	MOTA	2121	CA	VAL	303	35.059	-8.379	89.838	1.00 27.38	A
20	MOTA	2122	CB	VAL	303	33.547	-8.571	90.069	1.00 26.90	A
20										
	ATOM	2123	CG1	VAL	.303	33.052	-7.570	91.101	1.00 26.40	A
	ATOM	2124	CG2	VAI.	303	32.796	-8.428	88.770	1.00 29.98	A
							-9.341	88.744	1.00 30.52	A
	MOTA	2125	С	VAL	303	35.512				
	ATOM	2126	0	VAL	303	35.87 <i>7</i>	-10.477	89.035	1.00 31.69	A
25	MOTA	2127	N	GLU	304	35.491	-8.897	87.490	1.00 32.89	· A
23										
	ATOM	2128	CA	GLU	304	35.921	-9.750	86.389	1.00 35.74	. А
	ATOM	2129	CB	GLU	304	35.203	-9.374	85.094	1.00 37.37	A
	MOTA	2130	CG	GLU	304	33.689	-9.307	85.221	1.00 39.61	A
	MOTA	2131	CD	GLU	304	32.999	-9.146	83.876	1.00 42.09	A
30	ATOM	2132	OE1	GLU	304	33.515	-8.380	83.028	1.00 42.71	A
-			OE2		304	31.939	-9.775	83.671	1.00 41.78	A
	MOTA	2133								
	MOTA	2134	С	GLU	304	37.426	-9.604	86.206	1.00 37.86	A
	MOTA	2135	0	GLU	304	37.996	-10.078	85.227	1.00 37.10	A
								87.169	1.00 40.46	
26	ATOM	2136	N	ARG	305	38.054	-8.937			A
35	MOTA	2137	CA	ARG	305	39.496	-8.716	87.177	1.00 42.89	A ·
	ATOM	2138	CB	ARG	305	40.215	-10.025	87.534	1.00 45.84	A
							-10.328		1.00 50.55	A
	MOTA	2139	CG	ARG	305			89.040		
	MOTA	2140	CD	ARG	305	40.942	-9.222	89.795	1.00 55.95	A
	ATOM	2141	NE	ARG	305	40.641	-9.139	91.227	1.00 60.56	Α
40										
40	MOTA	2142	CZ	ARG	305	41.079	-9.988	92.154	1.00 62.46	A
	MOTA	2143	NH1	ARG	305	41.848	-11.016	91.816	1.00 63.45	A
	ATOM	2144	NH2		305	40.765	-9.793	93.431	1.00 62.35	A
	MOTA	2145	С	ARG	305	40.094	-8.101	85.913	1.00 43.03	A
	ATOM	2146	0	ARG	305	41.257	-8.337	85.585	1.00 42.44	A
45	ATOM	2147	N	THR	306	39.292	-7.300	85.218	1.00 43.37	A
7.7										
	MOTA	2148	CA	THR	306	39.728	-6.607	84.009	1.00 43.89	A
	MOTA	2149	CB	THR	306	38.553	-5.823	83.373	1.00 44.73	A
						37.525	-6.738	82.967	1.00 46.53	A
	MOTA	2150	OG1		306					
	MOTA	2151	CG2	THR	306	39.021	-5.031	82.173	1.00 44.99	A
50	MOTA	2152	С	THR	306	40.816	-5.616	84.428	1.00 43.35	A
							~4.883	85.405	1.00 44.14	A
	MOTA	2153	0	THR	306	40.648				
	MOTA	2154	N	PRO	307	41.944	-5.572	B3.696	1.00 42.66	A
	MOTA	·2155	CD	PRO	307	42.230	-6.282	82.436	1.00 43.08	A
								84.035	1.00 41.12	
	MOTA	2156	CA	PRO	307	43.039	-4.651			A
55	ATOM	2157	CB	PRO	307	44.109	-4.993	83.001	1.00 41.90	A
	MOTA	2158	CG	PRO	307	43.302	-5.410	81.811	1.00 42.89	A
	MOTA	2159	С	PRO	307	42.661	-3.165	84.023	1.00 39.78	A
	MOTA	2160	0	PRO	307	43.151	-2.384	84.847	1.00 38.90	A
	ATOM	2161	N	HIS	308	41.789	-2.773	83.099	1.00 36.76	A
60										
60	MOTA	2162	CA	HIS	308	41.373	-1.381	83.018	1.00 34.24	A
	MOTA	2163	CB	HIS	308	41.248	-0.946	81.558	1.00 35.68	A
		2164	CG	HIS	308	40.936	0.507	81.395	1.00 38.11	Ä
	ATOM									
	ATOM	2165	CD2	HIS	308	39.847	1.134	80.888	1.00 39.53	A
	ATOM	2166	ND1	HIS	308	41.794	1.503	81.809	1.00 38.73	A
65								81.565		
UJ	MOTA	2167		HIS	308	41.249	2.682		1.00 39.88	A
	MOTA	2168	NE2	HIS	308	40.067	2.486	81.006	1.00 40.19	A
	ATOM	2169	С	HIS	308	40.052	-1.120	83.737	1.00 31.65	A
	MOTA	2170	0	HIS	308	39.009	-1.661	83.362	1.00 32.49	A
	MOTA	2171	N	VAL	309	40.117	-0.282	84.769	1.00 26.89	A
70	MOTA	2172	CA	VAL	309	38.959	0.101	85.580	1.00 22.85	A
, 0										
	ATOM	2173	CB	VAL	309	39.298	-0.013	87.083	1.00 22.36	A
	MOTA	2174		VAL	309	38.091	0.351	87.922	1.00 22.91	A
									1.00 22.12	A
	MOTA	2175	CG2	VAL	309	39.765	-1.427	87.403	1.00 22.12	А

•	MOTA	2176	С	VAL	309	38.629	1.558	85.231	1.00 20.44	A
	ATOM	2177	0	VAL	309	39.450	2.446	85.433	1.00 19.97	A
	ATOM	2178	N	PRO	310	37.421	1.822	84.704	1.00 17.91	A
-	MOTA	2179	CD	PRO	310	36.413	0.834	84.277	1.00 14.72	A
5	ATOM	2180	CA	PRO	310	37.019	3.186	84.322	1.00 17.34	A
	ATOM	2181	CB	PRO	310	35.839	2.937	83.386	1.00 15.77	A
	ATOM	2182	CG	PRO	310	35.214	1.699	83.978	1.00 15.26	A
						36.689			1.00 16.65	A
	MOTA	2183	C	PRO	310		4.227	85.404		
	ATOM	2184	0	PRO	310	35.673	4.908	85.317	1.00 15.99	A
10	ATOM	2185	N	TYR	311	37.557	4.368	86.402	1.00 18.31	A
	ATOM	2186	·CA	TYR	311	37.346	5.335	87.485	1.00 18.33	A
	MOTA	2187	CB	TYR	311	38.549	5.374	88.430	1.00 18.13	A
	MOTA	2188	CG	TYR	311	38.826	4.115	89.209	1.00 20.50	A
	ATOM	2189	CD1	TYR	311	37.943	3.660	90.194	1.00 19.61	A
15	MOTA	2190	CE1	TYR	311	38.242	2.538	90.957	1.00 19.17	A
		2191	CD2	TYR	311	40.008	3.407	89.005	1.00 19.30	À
	MOTA									
	MOTA	2192	CE2	TYR	311	40.314	2.290	89.759	1.00 18.88	A
	MOTA	2193	CZ	TYR	311	39.432	1.860	90.732	1.00 20.10	A
	ATOM	2194	OH	TYR	311	39.754	0.749	91.480	1.00 23.13	A
20	MOTA	2195	Ċ	TYR	311	37.150	6.753	86.969	1.00 19.65	Ä
20										
	MOTA	2196	0	TYR	311	36.288	7.485	87.449	1.00 20.71	A
	MOTA	2197	N	ARG	312	37.967	7.140	85.995	1.00 19.46	A.
	MOTA	2198	CA	ARG	312	37.919	8.484	85.447	1.00 19.67	A
	MOTA	2199	CB	ARG	312	39.223	8.775	84.699	1.00 24.48	·A
25								85.534		
23	MOTA	2200	CG	ARG	312	40.470	8.521		1.00 31.49	A
	MOTA	2201	CD	ARG	312	41.737	8.793	84.742	1.00 38.21	A
	MOTA	2202	NE	ARG	312	41.948	10.223	84.543	1.00 41.59	A
	MOTA	2203	CZ	ARG	312	42.419	11.040	85.479	1.00 43.45	A
	MOTA	2204	NH1		312	42.733	10.564	86.678	1.00 43.96	A
20										
30	ATOM	2205	NH2		312	42.570	12.332	85.217	1.00 44.26	A
	MOTA	2206	С	ARG	312	36.736	8.826	84.547	1.00 17.18	A
	MOTA	2207	0	ARG	312	36.610	9.976	84.121	1.00 17.17	A
•	ATOM	2208	.N	GLU	313	35.856	7.869	84.262	1.00 14.11	A
								83.378	1.00 11.27	
25.	MOTA	2209	CA	GLU	313	34.729	8.178			A
35 ⁻	MOTA	-2210	CB	GLU	313	34.258	6.911	82.646	1.00 10.67	A
	MOTA	2211	CG	GLU	313	35.399	6.213	81.891	1.00 15.89	A
	MOTA	2212	CD	GLU	313	34.946	5.089	BO.956	1.00 19.42	A
		2213		GLU	313	35.821		80.519	1.00 20.64	A
	MOTA									
40	MOTA	2214	QE2	GLU	313	33.739	4.992	80.641	1.00 19.87	A
40	MOTA	2215	С	·GLU	313	33.554	8.893	84.048	1.00 9.14	A
	MOTA	2216	0	GLU	313	32.550	9.155	83.410	1.00 8.08	Α.
	MOTA	2217	N	SER	314	33.692	9.226	85.327	1.00 9.25	A.
	MOTA	2218	CA	SER	314	32.647	9.951	86.051	1.00 11.62	A
	MOTA	2219	CB	SER	314	31.508	9.011	86.467	1.00 14.09	A
45	MOTA	2220	OG	SER	314	31.812	8.354	87.688	1.00 14.04	A
	ATOM	2221	C	SER	314	33.233	10.604	87.298	1.00 11.57	A
		2222		SER	314	34.283	10.186	87.791	1.00 12.89	A
	MOTA		0							
	MOTA	2223	N	LYS	315	32.541	11.615	87.812	1.00 12.14	A
	MOTA	2224	CA	LYS	315	32.981	12.340	89.002	1.00 14.40	A
50	MOTA	2225	CB	LYS	315	32.082	13.556	89.246	1.00 17.33	A
	MOTA	2226	CG	LYS	315	32.015	14.559	88.105	1.00 19.52	A
		2227	CD	LYS	336	22 475	15.536	88.143	1.00 22.04	, A
	MOTA									
	MOTA	2228	CE	LYS	315	33.021	16.584	87.054	1.00 22.29	A
	MOTA	2229	NZ	LYS	315	32.991	15.922	85.724	1.00 25.05	A
55	MOTA	2230	С	LYS	315	32.952	11.461	90.253	1.00 14.36	A
	MOTA	2231	ŏ	LYS	315	33.899	11.459	91.042	1.00 15.78	A
	MOTA	2232	N	LEU	316	31.859	10.723	90.430	1.00 12.10	A
	MOTA	2233	CA	LEU	316	31.693	9.864	91.591	1.00 12.11	Α.
	MOTA	2234	CB.	LEU	316	30.346	9.132	91.521	1.00 11.47	A
60	MOTA	2235	CG	LEU	316	30.052	8.165	92.673	1.00 11.12	A
-		2236		LEU	316	29.755	8.941	93.947	1.00 10.52	Ä
	ATOM									
	ATOM	2237		LEU	316	28.867	7.294	92.313	1.00 9.92	A
	ATOM	2238	С	LEU	316	32.816	8.846	.91.790	1.00 12.47	A
	MOTA	2239	Ō	LEU	316	33.346	8.720	92.892	1.00 13.63	A
65		2240		THR	317	33.192	8.124	90.738	1.00 13.16	Ä
U)	MOTA		N							
	ATOM	2241	CA	THR	317	34.245	7.118	90.875	1.00 12.10	A
	MOTA	2242	CB	THR	317	34.132	6.031	89.783	1.00 9.66	A
	MOTA	2243		THR	317	34.077	6.642	88.496	1.00 9.89	A
	ATOM	2244		THR	317	32.870	5.200	89.994	1.00 10.70	Ä
70		2245								
70	MOTA		C	THR	317	35.674	7.681	90.923	1.00 12.84	A
	MOTA	2246	٥	THR	317	36.611	6.965	91.270	1.00 13.25	A
	MOTA	2247	Ν.	ARG	318	35.852	8.951	90.575	1.00 13.06	A
	ATOM	2248	CA	ARG	318	37.180	9.544	90.682	1.00 14.05	A
		,								••

	MOTA	2249	CB	ARG	318	37.326	10.780	89.796	1.00 15.43	A
	MOTA	2250	CG	ARG	318	37.417	10.473	88.319	1.00 20.15	A
	ATOM	2251	CD	ARG	318	37.526	11.755	87.527	1.00 22.93	A
	MOTA	2252	NE	ARG	318	38.747	12.468	87.865	1.00 27.97	Ä
5	MOTA			ARG	318	39.015	13.710	87.482	1.00 32.10	A
,		2253	CZ							
	MOTA	2254		ARG	318	38.138	14.383	86.747	1.00 32.47	A
	MOTA	2255	NH2	ARG	318	40.162	14.276	87.833	1.00 33.23	A
	ATOM	2256	С	ARG	318	37.281	9.948	92.138	1.00 13.35	A
	ATOM	2257	0	ARG	318	38.276	9.679	92.801	1.00 15.31	A
10	ATOM	2258	N	ILE	319	36.222	10.575	92.640	1.00 12.79	A
	ATOM	2259	CA	ILE	319	36.175	11.012	94.030	1.00 11.02	A
	ATOM	2260	СВ	ILE	319	34.837	11.727	94.322	1.00 9.24	A
	MOTA	2261		ILE	319	34.660	11.958	95.819	1.00 4.84	A
	ATOM	2262	CG1	ILE	319	34.786	13.047	93.561	1.00 9.26	A
15	ATOM	2263	CD1	ILE	319	33.431	13.786	93.692	1.00 9.14	A
	MOTA	2264	С	ILE	319	36.344	9.833	95.002	1.00 12.21	A
	ATOM	2265	ŏ	ILE	319	37.127	9.913	95.950	1.00 12.33	A
			N	LEU	320	35.627	8.739	94.752	1.00 10.74	Ä
	MOTA	2266								
20	MOTA	2267	CA	LEU	320	35.674	7.577	95.638	1.00 11.28	A
20	MOTA	2268	CB	LEU	320	34.240	7.142	95.965	1.00 8.50	A
	MOTA	2269	CG	LEU	. 320	33.364	8.196	96.642	1.00 11.65	A
	MOTA	2270	CD1	LEU	320	31.909	7.774	96.550	1.00 12.32	A
	MOTA	2271		LEU	320	33.794	8.390	98.090	1.00 7.79	A
	ATOM	2272	C	LEU	320	36.466	6.359	95.146	1.00 12.31	A
25										
23	MOTA	2273	0	LEU	320	36.276	5.254	95.658	1.00 10.52	A
	MOTA	2274	N	GLN	321	37.356	6.541	94.177	1.00 13.27	· A
	MOTA	2275	CA	·GLN	321	38.110	5.401	93.668	1.00 16.08	A
	MOTA	2276	CB	GLN	321	39.087	5.844	92.569	1.00 19.75	A
	ATOM	2277	CG	GLN	321	40.196	6.756	93.006	1.00 21.68	A
30	ATOM	2278	CD	GLN	321	41.079	7.139	91.840	1.00 25.85	A
	ATOM	2279		GLN	321	41.622	6.266	91.152	1.00 22.98	A
	MOTA	2280	NE2	GLN	321	41.228	8.450	91.602	1.00 26.88	A
	MOTA	2281	С	GLN	321	38.842	4.548	94.723	1.00 14.28	A
0.5	MOTA	2282	0	GLN	321	38.972	3.335	94.543	1.00 12.19	A
35	MOTA	2283	N	ASP	322	39.305	5.151	95.817	1.00 12.59	A ·
	MOTA	2284	CA	ASP	322	39.978	4.351	96.835	1.00 14.78	A
	ATOM	2285	CB	ASP	322	40.769	5.230	97.811	1.00 17.14	A
	ATOM	2286	CG	ASP	322	41.787	4.426	98.620	1.00 18.36	A
40	MOTA	2287		ASP	322	42.588	3.692	98.003	1.00 19.34	A
40	MOTA	2288		ASP	322	41.791	4.521	99.865	1.00 19.68	A
	ATOM	2289	С	ASP	322	38.988	3.473	97.609	1.00 15.66	A
	MOTA	2290	0	ASP	322	39.384	2.598	98.384	1.00 17.16	A
	ATOM	2291	N	SER	323	37.697	3.696	97.386	1.00 16.21	A
	MOTA	2292	CA	SER	323	36.657	2.915	98.047	1.00 16.47	A
45	ATOM	2293	СВ	SER	323	35.436	3.795	98.343	1.00 13.71	A
73										
	MOTA	2294	OG	SER	323	35.749	4.804	99.284	1.00 11.67	A
	MOTA	2295	С	SER	323	36.247	1.735	97.166	1.00 18.02	A
	ATOM	2296	0	SER	323	35.459	0.876	97.574	1.00 18.75	A
	MOTA	2297	N	LEU	324	36.795	1.696	95.956	1.00 18.69	A
50	MOTA	2298	CA	LEU	324	36.495	0.635	95.009	1.00 19:76	A
	ATOM	2299	CB	LEU	324	35.782	1.225	93.789	1.00 19.37	A
	ATOM	2300	CG	LEU	324	34.461	1.920	94.127	1.00 19.69	A
	MOTA	2301		LEU	324	34.028	2.781	92.973	1.00 22.50	A
E E	MOTA	2302		LEU	324	33.394	0.887	94.449	1.00 20.33	A
55	MOTA	2303	С	LEU	324	37.789	-0.045	94.591	1.00 21.46	A
	ATOM	2304	0	LEU	324	38.427	0.353	93.618	1.00 23.00	A
	MOTA	2305	N	GLY	325	38.174	-1.074	95.341	1.00 22.77	A
	MOTA	2306	CA	GLY	325	39.398	-1.794	95.047	1.00 21.76	Ä
		2307			325	40.620		95.516	1.00 24.37	A
60	MOTA		C	GLY			-1.028			
OU	MOTA	2308	0	GLY	325	41.718	-1.239	95.005	1.00 24.93	A
	MOTA	2309	N	GLY	326	40.428	-0.132	96.484	1.00 24.40	A
	MOTA	2310	CA	GLY	326	41.526	0.663	97.002	1.00 24.15	A
	MOTA	2311	С	GLY	326	41.897	0.284	98.424	1.00 26.42	A _.
	ATOM	2312	ō	GLY	326	41.656	-0.840	98.856	1.00 25.60	A
65	MOTA	2313	N	ARG	327	42.470	1.220	99.168	1.00 25.86	A
55			CA							
	MOTA	2314		ARG	327	42.875		100.528	1.00 28.96	A
	MOTA	2315	CB	ARG	327	44.219	1.593		1.00 32.07	· А
	MOTA	2316	CG	ARG	327	45.329	1.220	99.853	1.00 37.14	A
	MOTA	2317	CD	ARG	327	46.714	1.483	100.432	1.00 42.74	A
70	MOTA	2318	NE	ARG	327	47.800	1.031	99.556	1.00 47.24	A
	ATOM	2319	CZ	ARG	327	48.286	1.730	98.530	1.00 49.78	A
	MOTA	2320		ARG	327	47.787	2.926	98.237	1.00 50.77	A
	ATOM	2321			327					
	AT OU	2.7.E.T	MUZ	ARG	321	49.286	1.245	97.805	1.00 49.64	A

	ATOM	2322		ARG	327	41.831	1.320	101.569	1.00 28.96	A
			C							
	ATOM	2323	0	ARG	327	42.157		102.731	1.00 28.88	A
	ATOM	2324	N	THR	328	40.573		101.151	1.00 27.38	A
_	ATOM	2325	CA	THR	328	39.499	1.775	102.064	1.00 23.77	A
5	MOTA	2326	CB	THR	328	38.678	2.944	101.488	1.00 24.66	A
	ATOM	2327		THR	328	39.529	4.088	101.344	1.00 25.37	A
	ATOM	2328	CG2	THR	328	37.510		102.409	1.00 23.54	A
					328					
	ATOM	2329	C	THR		38.556		102.353	1.00 20.49	A
10	MOTA	2330	0	THR	328	38.287		101.480	1.00 19.13	A
1.0	ATOM	2331	N	ARG	329	38.072	0.532	103.588	1.00 17.06	A.
	ATOM	2332	·CA	ARG	329	37.139	-0.522	103.954	1.00 15.33	A
	ATOM	2333	СВ	ARG	329	37.126	-0.768	105.465	1.00 14.79	A
	ATOM	2334	CG	ARG	329	36.035		105.878	1.00 15.14	A
•	ATOM	2335	CD	ARG	329	35.989		107.370	1.00 17.09	A
15	ATOM		NE	ARG	329					
13		2336				34.897		107.655	1.00 21.72	A
	ATOM	2337	CZ	ARG	329	34.688		108.819	1.00 22.49	A
	MOTA	2338	NH1		329	35.504		109.841	1.00 20.08	A
	ATOM	2339	NH2	ARG	329	33.646		108.958	1.00 22.92	A
	ATOM	2340	С	ARG	329	35.783	-0.001	103.539	1.00 14.65	A
20	ATOM	2341	0	ARG	329	35.352	1.046	104.030	1.00 15.12	A
	ATOM	2342	N	THR	330	35.107		102.640	1.00 12.06	A
	ATOM	2343	CA	THR	330	33.809		102.224	1.00 14.04	A.
	ATOM	2344	CB	THR	330	33.837		100.782	1.00 15.17	A
25	MOTA	2345	OG1		330	33.694	-0.735	99.847	1.00 18.22	· A
23	ATOM	2346	CG2	THR	330	35.147		100.513	1.00 14.36	A
	MOTA	2347	С	THR	330	32.707		102.323	1.00 13.65	A _.
	MOTA	2348	0	THR	330	32.936	-2.459	102.140	1.00 13.67	A
	MOTA	2349	N	SER	331	31.509	-0.786	102.637	1.00 12.70	A
	MOTA	2350	CA	SER	331	30.340	-1.627	102.740	1.00 10.49	A
30	MOTA	2351	СВ	SER	331	29.830		104.177	1.00 12.02	A
	ATOM	2352	OG	SER	331	30.860		105.072	1.00 18.36	A
	ATOM	2353	č	SER	331	29.259		101.830	1.00 10.83	Ä
	MOTA	2354	0	SER	331	29.235		101.555	1.00 8.62	A
25.	ATOM	2355	N	ILE	332	28.376		101.349	1.00. 9.52	A
35 ·	MOTA .	2356	ÇA	ILE	332	27.288		100.511	1.00 9.50	A
	ATOM	2357	CB	ILE	332	27.374	-2.038	99.089	1.00 10.70	A
	MOTA	2358	CG2	ILE	332	26.143	-1.622	98.287	1.00 8.05	A
	MOTA	2359	CG1	ILE	332	28.650	-1.560	98.394	1.00 9.17	A
	ATOM	2360		ILE	332	28.773	-2.094	96.975	1.00 5.23	A
40	ATOM	2361	c	ILE	332	25.993		101.138	1.00 9.51	A
40		2362		ILE	332	25.843				
	ATOM		0					101.413	1.00 9.19	A
	ATOM	2363	N	ILE	333	25.074		101.391	1.00 9.81	A
	ATOM	2364	CA	ILE	333	23.773		101.942	1.00 8.92	A
45	ATOM	23,65	CB	ILE	333	23.335		103.103	1.00 8.82	A
45	ATOM	2366	CG2	ILE	333	21.967	-0.863	103.614	1.00 7.93	A
	MOTA	2367	CG1	ILE	333	24.316	-0.548	104.272	1.00 6.76	A
	ATOM	2368	CD1	ILE	333	24.028	0.448	105.387	1.00 2.97	A
	ATOM	2369	С	ILE	333	22.777		100.797	1.00 9.34	A
	ATOM	2370	ō.	ILE	333	22.483		100.347	1.00 6.58	A
50	ATOM	2371	N	ALA	334	22.294		100.303	1.00 9.13	Ä
50		2372				21.325				
	MOTA		CA	ALA	334		-2.370	99.215	1.00 8.43	A
	MOTA	2373	CB	ALA	334	21.543	-3, 582	98.318	1.00 6.36	A
	ATOM	2374	С	ALA	334	19.903	-2.381	99.807	1.00 8.65	A
	MOTA	2375	0	ALA	334	19.555	-3.232	100.634	1.00 6.98	A
55	ATOM	2376	N	THR	335	19.089	-1.419	99.398	1.00 8.61	A
	ATOM	2377	CA	THR	335	17.727	-1.334	99.899	1.00 8.77	A
	MOTA	2378	CB	THR	335	17.375		100.290	1.00 7.57	A
	ATOM	2379		THR	335	17.538	0.949	99.157	1.00 8.21	A
					335					
60	MOTA	2380		THR		18.276		101.398	1.00 7.82	A
UU	MOTA	2381	C	THR	335	16:729	-1.820	98.863	1.00 8.70	A
	MOTA	2382	0	THR	335	16.855	-1.530	97.671	1.00 8.21	A
	ATOM	2383	N	ILE	336	15.735	-2.560	99.338	1.00 8.74	A
	MOTA	2384	CA	ILE	336	14.717	-3.124	98.469	1.00 10.87	A
	MOTA	2385	CB	ILE	336	14.998	-4.613	98.216	1.00 10.46	A
65	ATOM	2386		ILE	336	16.353	-4.769	97.532	1.00 8.62	A
	ATOM	2387		ILE	336	14.943	-5.379	99.543	1.00 10.60	Ä
	MOTA	2388		ILE	336	14.993	-6.921	99.386	1.00 10.00	
										A
	MOTA	2389	C	ILE	336	13.291	-2.995	99.004	1.00 12.03	A
70	MOTA	2390	0	ILE	336	13.069		100.204	1.00 12.49	A
70	MOTA	2391	N	SER	337	12.331	-3.056	98.089	1.00 13.93	Α
	MOTA	2392	CA	SER	337	10.918	-2.969	98.426	1.00 13.83	Α
	MOTA	2393	CB	SER	337	10.180	-2.154	97.359	1.00 14.05	A
	MOTA	2394	OG	SER	337	8.790	-2.436	97.350	1.00 13.32	A
										••

	ATOM	2395	С	SER	337	10.371	-4.386	98.464	1.00 14.60	A
		2396	ŏ	SER	337	10.829	-5.250	97.717	1.00 14.95	A
	ATOM									
	ATOM	2397	N	PRO	338	9.398	-4.652	99.350	1.00 15.93	· A
-	MOTA	2398	CD	PRO	338	8.967		100.483	1.00 16.39	A
5	MOTA	2399	CA	PRO	338	8.809	-5.990	99.451	1.00 15.42	A
	MOTA	2400	CB	PRO	338	8.461	-6.088	100.921	1.00 15.52	A
	MOTA	2401	CG	PRO	338	7.930		101.176	1.00 17.59	A
	MOTA	2402	c	PRO	338	7.564	-6.138	98.576	1.00 15.52	A
10	MOTA	2403	0	PRO	338	6.929		98.571	1.00 17.10	A
10	MOTA	2404	N	ALA	339	7.212	-5.091	97.841	1.00 15.73	A
	ATOM	2405	CA	ALA	339	6.023	-5.122	96.989	1.00 17.08	· A
	ATOM	2406	CB	ALA	339	5.494	-3.699	96.765	1.00 13.90	A
	ATOM	2407	С	ALA	339	6.255	-5.793	95.647	1.00 17.79	A
	ATOM	2408		ALA	339	7.290	-5.586	95.010	1.00 18.27	A
15	ATOM	2409	N	SER	340	5.270	-6.575	95.210	1.00 19.26	A
10					340 .	5.339	-7.280	93.933	1.00 20.19	A
	MOTA	2410	CA	SER						
	MOTA	2411	CB	SER	340	4.088	-8.151	93.741	1.00 21.56	À
	MOTA	2412	OG	SER	340	2.909	-7.370	93.812	1.00 24.50	A
	ATOM	2413	С	SER	340	5.495	-6.340	92.736	1.00 18.83	A
20	MOTA	2414	0	SER	340	5.977	-6.755	91.687	1.00 17.98	A
	ATOM	2415	N	LEU	341	5.083	-5.084	92.883	1.00 19.49	A
	ATOM -	2416	CA	LEU	341	5.212	-4.114	91.793	1.00 21.42	A
	ATOM	2417	CB	LEU	341	4.539	-2.787	92.159	1.00 24.24	A
25	ATOM	2418	CG	LEU	341	3.056	-2.763	92.528	1.00 30.57	A
25	ATOM	2419		LEU	341	2.838	-3.310	93.952	1.00 30.86	· A
	MOTA	2420	CD2	LEU	341	2.563	-1.325	92.435	1.00 32.23	. А
	ATOM	2421	С	. LEU	341	6.678	-3.821	91.452	1.00 20.58	A
	MOTA	2422	0	LEU	341	7.017	-3.528	90.308	1.00 20.62	A
	ATOM	2423	N	ASN	342	7.544	-3.905	92.455	1.00 19.46	A
30	ATOM	2424	CA	ASN	342	8.958	-3.620	92.267	1.00 18.47	A
	ATOM	2425	CB	ASN	342	9.471	-2.863	93.485	1.00 17.34	Ä
	MOTA	2426	CG	ASN	342	8.662	-1.618	93.763	1.00 16.86	Α
	MOTA	2427		ASN	342.	8.564	-0.730	92.916	1.00 18.67	A
0.5	MOTA	2428	ND2	ASN	342	8.070	-1.546	94.944	1.00 15.28	A
35	ATOM	2429	С	ASN	342	9.795	-4.871	92.041	1.00 18.85	Α .
	MOTA	2430	0	ASN	342	10.988	-4.893	92.351	1.00 17.91	A
	MOTA	2431	N	LEU	343	9.170	-5.908	91.493	1.00 17.20	A
	ATOM	2432	CA	LEU	343	9.863	-7.163	91.252	1.00 17.19	A
40	ATOM	2433	CB	LEU	343	8.917	-8.179	90.596	1.00 13.78	Ą
40	ATOM	2434	CG	LEU	343	9.593	-9.472	90.107	1.00 14.61	Ä
	ATOM	2435	CD1	LEU	343	10.343	-10.143	91.269	1.00 10.55	A
	ATOM	2436	CD2	LEU	343	8.554	-10.415	89.499	1.00 13.10	A
	ATOM	2437	С	LEU	343	11.115	-7.020	90.399	1.00 17.48	A
	MOTA	2438	0	LEU	343	12.211	-7.377	90.829	1.00 17.34	A
45	ATOM	2439	N	GLU	344	10.946	-6.514	89.184	1.00 19.72	A
	MOTA	2440	CA	GLŲ	344	12.063	-6.358	88.263	1.00 20.96	A
			CB	GLU		11.598	-5.684	86.969	1.00 24.20	
	MOTA	2441			344					A
	MOTA	2442	CG	GLU	344	12.675	-5.635	85.887	1.00 32.62	A
50	MOTA	2443	CD	GĽU	344	12.213	-4.959	84.599	1.00 38.13	A
50	ATOM	2444	OE1	GLU	344	12.908	-5.115	83.566	1.00 40.01	A
	ATOM	2445	OE2	GLU	344	11.165	-4.270	84.617	1.00 41.47	A
	ATOM	2446	С	GLU	344	13.208	-5.561	88.883	1.00 20.19	A
	ATOM	2447	0	GLU	344	14.371	-5.957	88.791	1.00 20.32	A
	MOTA	2448	N	GLU	345	12.883	-4.441	89.518	1.00 17.74	A
55	ATOM	2449	CA	GLU	345	13.909	-3.615	90.130	1.00 18.84	A
55	ATOM	2450	CB	GLU	345	13.335	-2.240	90.496	1.00 21.25	Ä
	MOTA	2451	CG	GLU	345	13.076	-1.356	89.281	1.00 24.52	A
	MOTA	2452	CD	GLU	345	14.348	-1.036	88.492	1.00 27.03	A
	MOTA	2453	OE1	GLU	345	14.232	-0.592	87.325	1.00 29.83	A
60	ATOM	2454	OE2	GLU	345	15.462	-1.216	89.036	1.00 27.61	A
	MOTA	2455	С	GLU	345	14.555	-4.270	91.346	1.00 16.79	A
	ATOM	2456	ō	GLU	345	15.762	-4.143	91.554	1.00 17.33	A
	ATOM	2457	N	THR	346	13.760	-4.978	92.140	1.00 14.42	Ä
65	MOTA	2458	CA	THR	346	14.286	-5.649	93.316	1.00 14.40	A
O)	MOTA	2459	CB	THR	346	13.160	-6.304	94.138	1.00 15.55	Α
	MOTA	2460		THR	346	12.399	-5.285	94.801	1.00 13.04	A
	MOTA	2461	CG2	THR	346	13.735	-7.255	95.171	1.00 15.14	A
	MOTA	2462	С	THR	346	15.302	-6.705	92.896	1.00 14.50	A
	MOTA	2463	0	THR	346	16.294	-6.922	93.590	1.00 13.63	A
70	ATOM	2464	N	LEU	347	15.061	-7.362	91.763	1.00 14.51	A
	ATOM	2465	CA	LEU	347	16.005	-8.357	91.269	1.00 15.49	Ä
	MOTA	2466	CB	LEU	347	15.369	-9.222	90.167	1.00 15.24	A
	MOTA	2467	CG	LEU	347	14.220	-10.158	90.571	1.00 15.51	A

•	MOTA	2468	CD1	LEU	347	13.712	-10.902	89.351	1.00 11.90	A
	MOTA	2469	CD2	LEU	347	14.687	-11.142	91.627	1.00 13.17	A
	ATOM	2470	С	LEU	347	17.267	-7.666	90.734	1.00 16.52	A
	ATOM	2471	ŏ	LEU	347	18.376	-8.175	90.908	1.00 18.79	A
5	ATOM		N	SER	348	17.111	-6.513	90.088	1.00 15.74	A
,		2472								
	MOTA	2473	CA	SER	348	18.274	-5.795	89.567	1.00 16.97	A
	MOTA	2474	CB	SER	348	17.857	-4.502	88.872	1.00 17.03	A
	MOTA	2475	OG	SER	348	17.008	-4.785	87.780	1.00 23.78	A
	ATOM	2476	С	SER	348	19.199	-5.438	90.712	1.00 16.29	A
10	ATOM	2477	õ	SER	348	20.415	-5.668	90.655	1.00 17.03	A
10	MOTA	2478	.N	THR	349	18.603	-4.864	91.751	1.00 13.43	A
	MOTA	2479	CA	THR	349	19.341	-4.452	92.925	1.00 12.53	A
	ATOM	2480	CB	THR	349	18.400	-3.808	93.953	1.00 11.53	A
	MOTA	2481	OG1	THR	349	17.883	-2.583	93.416	1.00 12.14	A
15	ATOM	2482	CG2	THR	349	19.143	-3.512	95.243	1.00 8.21	A
-	ATOM	2483	C	THR	349	20.074	-5.624	93.563	1.00 12.73	A
	ATOM	2484	ŏ	THR	349	21.292	-5.590	93.732	1.00 10.74	A
									1.00 14.33	A
	ATOM	2485	N	LEU	350	19.325	-6.660	93.916		
20	MOTA	2486	CA	LEU	350	19.923	-7.830	94.532	1.00 16.65	A
20	ATOM	2487	СВ	LEU	350	18.855	-8.892	94.803	1.00 14.51	A
	ATOM	2488	CG	LEU	350	17.916	-8.537	95.960	1.00 13.75	A
	MOTA	2489	CD1	LEU	350	16.780	-9.516	96.035	1.00 10.80	A
	ATOM	2490		LEU	350	18.703	-8.526	97.258	1.00 15.25	A ·
	ATOM	2491	c	LEU	350	21.033	-8.400	93.660	1.00 17.62	·A
25										
23	MOTA	2492	0	LEU	350	22.116	-8.695	94.148	1.00 19.69	A
	MOTA	2493	N	GLU	351	20.774	-8.540	92.368	1.00 18.77	A
	MOTA	2494	CA	GLU	351	21.783	-9.078	91.466	1.00 20.26	A
	MOTA	2495	CB	GLU	351	21.203	-9.215	90.061	1.00 23.16	A
	MOTA	2496	CG	GLU	351	21.961	-10.194	89.186	1.00 31.07	A
30	ATOM	2497	CD	GLU	351	21.645	-11.652	89.508	1.00 35.15	A
50	MOTA	2498		GLU	351	22.421	-12.531	89.070	1.00 37.94	Ä
			-							
	MOTA	2499		GLU	351	20.621	-11.921	90.180	1.00 35.11	A
	MOTA	2500	C	GLU	351	23.030	-8.181	91.440	1.00 18.73	A
~ ~	MOTA	2501	0	GLU	351	24.163	-8.662	91.407	1.00 18.86	A
35·	ATOM .	.2502	N	TYR	352	22.810	-6.873	91.463	1.00 18.82	A
	MOTA	2503	CA	TYR	352	23.893	-5.898	91.443	1.00 16.90	A
	MOTA	2504	СВ	TYR	352	23.304	-4.500	91.261	1.00 17.28	A
	ATOM	2505	CG	TYR	352	24.306	-3.374	91.118	1.00 15.30	A
40	MOTA	2506		TYR	352	24.940	-2.833	92.227	1.00 12.89	A
40	MOTA	2507		TYR	352	25.779	-1.740	92.100	1.00 15.82	A
	ATOM	2508	CD2	TYR	352	24.550	-2.798	89.869	1.00 15.34	A
	ATOM	2509	CE2	TYR	352	25.382	-1.712	89.731	1.00 14.65	A
	ATOM	2510	CZ	TYR	352	25.989	-1.180	90.848	1.00 15.26	A
	ATOM	2511	ОН	TYR	352	26.767	-0.050	90.715	1.00 17.76	A
45	ATOM	2512	C	TYR	352	24.688	-5.973	92.733	1.00 16.43	Ä
43										
	MOTA	2513	0	TYR	352	25.917	-5.964	92.715	1.00 17.51	A
	MOTA	2514	N.	ALA	353	23.989	-6.065	93.855	1.00 15.81	Ά
	ATOM	2515	CA	ALA	353	24.658	-6.137	95.145	1.00 16.65	A
	ATOM	2516	CB	ALA	353	23.646	-5.931	96.269	1.00 15.23	A
50	ATOM	2517	С	ALA	353	25.405	-7.458	95.350	1.00 17.40	A
	ATOM	2518	ŏ	ALA	353	26.412	-7.497	96.050	1.00 18.96	A
	MOTA	2519	N	HIS	354	24.916	-8.535	94.744	1.00 18.26	A
	MOTA	2520	CA	HIS	354	25.555	-9.838	94.883	1.00 19.76	A
	MOTA	2521	СВ	HIS	354	24.676	-10.932	94.266	1.00 19.50	A
55	MOTA	2522	CG	HIS	354	25.143	-12.324	94.566	1.00 21.21	A
	ATOM	2523	CD2	HIS	354	25.758	-13.246	93.786	1.00 20.11	A
	MOTA	2524	ND1	HIS	354	25.032	-12.894	95.817	1.00 20.61	A
	ATOM	2525		HIS	354		-14.105	95.796	1.00 20.62	Α,
	ATOM	2526		HIS	354		-14.342	94.576	1.00 20.83	A
60 -										
OV .	ATOM	2527	C	HIS	354	26.936	-9.842	94.224	1.00 21.08	A
	MOTA	2528	0	HIS	354		-10.313	94.816	1.00 22.05	A
	MOTA	2529	N	ARG	355	27.027	-9.314	93.004	1.00 22.49	A
	MOTA	.2530	CA	ARG	355	28.308	-9.256	92.292	1.00 24.62	A
	MOTA	2531	СВ	ARG	355	28.153	-8.619	90.905	1.00 25.83	Α
65	ATOM	2532	CG	ARG	355	27.358	-9.413	89.894	1.00 29.38	A
55								88.535	1.00 32.38	
	MOTA	2533	CD	ARG	355	27.482	-8.762			A
	MOTA	2534	NE	ARG	355	27.233	-7.326	88.622	1.00 37.22	A
	MOTA	2535	CZ	ARG	355	27.902	-6.412	87.924	1.00 40.93	A
	MOTA	2536	NH1	ARG	355	28.860	-6.797	87.087	1.00 41.58	A
70	ATOM	2537	NH2	ARG	355	27.624	-5.117	88.066	1.00 39.72	A
	ATOM	2538	С	ARG	355	29.352	-8.447	93.054	1.00 24.34	A
	ATOM	2539	ŏ	ARG	355	30.523	-8.821	93.098	1.00 25.69	Ä
									1.00 23.36	
	ATOM	2540	N	ALA	356	28.923	-7.332	93.640	1.00 23.30	A

	MOTA	2541	CA	ALA	356	29.814	-6.447	94.387	1.00 22.82	A
	MOTA	2542	CB	ALA	356	29.016	-5.295	94.985	1.00 20.20	A ·
	MOTA	2543	C	ALA	356	30.603	-7.161	95.484	1.00 23.12	` A
_	MOTA	2544	0	ALA	356	31.708	-6.751	95.820	1.00 20.69	A
5	MOTA	2545	N	LYS	357	30.030	-8.222	96.047	1.00 24.95	A
	ATOM	2546	CA	LYS	357	30.695	-8.981	97.111	1.00 26.72	A
	ATOM	2547	CB	LYS	357	29.849	-10.195	97.497	1.00 25.95	A
	ATOM	2548	CG	LYS	357	28.570	-9.854	98.232	1.00 27.20	A
10	ATOM	2549	CD	LYS	357		-11.052	98.293	1.00 28.41	A
10	MOTA	2550	CE	LYS	357		-12.220	99.024	1.00 29.67	A
	MOTA	2551	NZ	LYS	357		-13.483	98.790	1.00 30.65	A
	MOTA	2552	¢	LYS	357	32.099	-9.453	96.733	1.00 27.68	A
	ATOM	2553	0	LYS	357	32.968	-9.595	97.601	1.00 26.10	A
15	ATOM	2554	N	ASN	358	32.312	-9.691	95.438	1.00 28.56	A
15	ATOM	2555	CA	ASN	358		-10.177	94.925	1.00 28.98	A
	ATOM	2556	CB	ASN	358		-10.897	93.597	1.00 31.13	A
	ATOM	2557	CG	ASN	358		-12.071	93.735	1.00 34.60	A
	ATOM	2558		ASN	358	32.743	-13.071	94.375	1.00 37.20	A
20	ATOM	2559 2560		asn Asn	358 358	34.676	-11.952 -9.118	93.145 94.751	1.00 33.97 1.00 27.98	A A
20	ATOM ATOM	2561	C O	ASN	358	35.784	-9.426	94.316	1.00 27.98	A
	MOTA	2562	N	ILE	359	34.364	-7.871	95.079	1.00 25.92	Ä
	ATOM	2563	CA	ILE	359	35.350	-6.811	94.957	1.00 24.09	Ä
	ATOM	2564	CB	ILE	359	34.673	-5.429	94.910	1.00 21.25	A
25	ATOM	2565		ILE	359	35.727	-4.329	94.867	1.00 19.17	A
	MOTA	2566		ILE	359	33.748	-5.367	93.689	1.00 19.08	A
	ATOM	2567		ILE	359	32.909	-4.109	93.597	1.00 18.25	A
	MOTA	2568	С	ILE	359	36.290	-6.906	96.155	1.00 25.26	A
	MOTA	2569	0	ILE	359	35.847	-7.076	97.290	1.00 23.96	A
30	ATOM	2570	N	LEU	360	37.588	-6.817	95.897	1.00 27.58	A
	MOTA	2571	CA	LEU	360	38.578	-6.917	96.963	1.00 32.07	A
	MOTA	2572	CB	LEU	360	39.478	-8.137	96.722	1.00 34.40	A
	ATOM	2573	CG	LEU	360.	40.711	-8.333	97.613	1.00 36.57	A
~~	ATOM	2574	CD1	LEU	360	40.309	-8.930	98.961	1.00 37.87	A
35	MOTA	2575	CD2	LEU	360	41.687	-9.265	96.913	1.00 38.48	Α
	MOTA	2576	С	LEU	360	39.438	-5.665	97.033	1.00 33.54	A
	MOTA	2577	0	LEU	360	39.905	-5.174	96.008	1.00 32.97	A
	MOTA	2578	N	ASN	361	39.635	-5.132	98.234	1.00 35.62	A
40	ATOM	2579	CA	ASN	361	40.485	-3.962	98.372	1.00 39.86	A
40	ATOM	2580	CB	ASN	361	39.649	-2.672	98.395	1.00 41.32	À
	ATOM	2581	CG	ASN	361	38.490	-2.732	99.345	1.00 42.28	A
	MOTA	2582		ASN	361	37.523	-1.985	99.203	1.00 42.60	A
	MOTA	2583		ASN	361	38.578		100.330	1.00 45.41	A
45	ATOM ATOM	2584 2585	0	asn asn	361 361	41.439 41.180	-4.056 -4.768	99.565 100.532	1.00 41.68 1.00 41.90	A A
73	ATOM	2586	Ŋ	LYS	362	42.560	-3.348	99.446	1.00 41.90	A
	MOTA	2587	CA	LYS	362	43.643		100.432	1.00 44.89	A
	MOTA	2588	CB	LYS	362	43.106		101.870	1.00 45.91	Ä
	ATOM	2589	CG	LYS	362	42.518		102.353	1.00 44.95	Ä
50	ATOM	2590	CD	LYS	362	42.184		103.841	1.00 44.77	A
	MOTA	2591	CE	LYS	362	43.444		104.701	1.00 44.68	Ā
	MOTA	2592	NZ	LYS	362	44.224	-0.795	104.523	1.00 44.09	A
	ATOM	-2593	С	LYS	362	44.576		100.173	1.00 48.88	A
	ATOM	2594	0	LYS	362	44.928		101.141	1.00 50.91	A
55	MOTA	2595	ОХТ	LYS	362	44.955	-4.700	98.992	1.00 49.21	A
	ATOM	2596	MG	MG	603	16.038	9.381	98.154	1.00 22.45	
	ATOM	2597	PB	ADP	601	14.871	6.512	98.896	1.00 9.83	ADP
	ATOM	2598		ADP	601	14.389	7.073	97.604	1.00 11.43	ADP
~	ATOM	2599		ADP	601	15.417	5.029	98.682	1.00 12.43	ADP
60	ATOM	2600		ADP	601	15.921	7.374	99.491	1.00 9.54	ADP
	ATOM	2601	PA	ADP	601	13.343		101.254	1.00 13.34	ADP
	ATOM	2602		ADP	601	14.336		102.280	1.00 14.02	ADP
	ATOM	2603		ADP	601	13.336		101.013	1.00 12.22	ADP
65	MOTA	2604		ADP	601	13.676	6.373	99.912	1.00 11.56	ADP
05	MOTA	2605		ADP ADP	601	11.879		101.742	1.00 16.31	ADP
	MOTA	2606			601	10.894		101.155	1.00 16.15	ADP
	MOTA	2607 2608		ADP ADP	601 601	9.662 9.712		102.132	1.00 18.96 1.00 19.62	ADP
	ATOM ATOM	2608		ADP	601	9.712		102.849	1.00 19.62	ADP ADP
70	ATOM	2610		ADP	601	8.406		103.229	1.00 18.80	ADP
, ,	MOTA	2611		ADP	601	10.188		103.431	1.00 22.72	ADP
	MOTA	2612		ADP	601	9.655		105.672	1.00 21.78	ADP
	ATOM	2613		ADP	601	9.788		104.281	1.00 19.08	ADP

												•	
•	MOTA	2614	N9	ADP	601	10	.778	3.943	104.795	1.00	19.36	ADP	
	ATOM	2615	C8	ADP	601		. 895	3.536	104.137	1.00		ADP	
	MOTA	2616	N7	ADP	601	12	. 535	2.641	104,859	1.00	19.29	ADP	
_	MOTA	2617	C5	ADP	601	11	. 874	2.450	105.961	1.00	20.60	ADP	
5	ATOM	2618	C6	ADP	601	12	.043	1.649	107.091	1.00	20.38	ADP	
	MOTA	2619	N6	ADP	601	13	. 085	0.825	107.178	1.00	20.28	ADP	
	MOTA	2620	N1	ADP	601	11	.118	1.701	108.120	1.00	22.79	ADP	
	MOTA	2621	C2	ADP	601	10	.028	2.524	108.081	1.00	22.78	ADP	
	MOTA	2622	N3	ADP	601	9.	. 854	3.302	106.988	1.00	20.98	ADP	
10	ATOM	2623	C4	ADP	601	10	.736	3.301	105.936	1.00	20.39	ADP	
	MOTA	2859	· C1	5-2b	2	19.	.000	14.175	112.199	1.00	28.18	5-21	9
	ATOM	2860	C2	5-2b	2	18.	061		111.340	1.00		5-21	
	ATOM	2861	C3	5-2b	2	17.	.078	12.651	111.895	1.00	28.56	5-21	
	ATOM	2862	C4	5-2b	2 .		.088	12.427	113.305	1.00		5-21	
15	ATOM	2863	C5	5-2b	2	18	039		114.157	1.00		5-2h	
	MOTA	2864	C6	5-2b	2		015		113.622	1.00		5-2h	
•	MOTA	2865	C7	5-2b	2		128		109.878	1.00		5-21	
	MOTA	2866	N8	5-2b	2		295		109.173	1.00		5-21	
	MOTA	2867	C9	5-2b	2	20.	221		108.603	1.00		5-2k	
20	MOTA	2868	N10	5-2b	2		947		108.469	1.00		5-21	
	MOTA	2869		5-2b	2		661		108.801	1.00		5-21	
	MOTA	2870		5-2b	2		708		109.368	1.00		5-21	
	MOTA	2871	013	5-2b	2		238		113.800	1.00		5-21	
	MOTA	2872		5-2b	2		264		109.536	1.00		5-21	
25	MOTA	2873		5-2b	2		927		109.475	1.001		5-21	
	ATOM	2874		5-2b	2		579		109.627	1.00		5-21	
	MOTA	2875		5-2b	2.		646		109.575	1.00		5-21	
	MOTA	2876	C18	5-2b	2		590		108.468	1.00		5-21	
	MOTA	2877	019	5-2b	2		462		109.721		72.50	5-21	
30	MOTA	2878		5-2b	2		688		108.038	1.00		5-21	
	ATOM	2624	0	нон	1		805	10.444	96.618	1.00	3.59	s	
	ATOM	2625	0	нон	6		478	8.895	97.954	1.00		s	
	ATOM	2626	Ō	нон	7		678		114.749	1.00	5.86	s	
	ATOM	2627	Ó	нон	8		946	-1.691	94.899	1.00	5.80	Š	
35	ATOM	2628	0	нон	11		220	17.072	106.339	1.00	1.72	s	
	ATOM	2629	0	нон	13		805	10.449	99.917	1.00	8.07	s	
	ATOM	2630	0	HOH	16	13.	355	-2.493	95.064	1.00	7.03	s	
	MOTA	2631	Ó	нон	19		262		111.999	1.00	8.18	š	
	ATOM	2632	0	нон	20		684		117.065	1.00		s	
40	ATOM	2633	Ó	нон	25		216	2.976	93.758	1.00		s	
	MOTA	2634	0	нон	27		932		102.192	1.00	7.13	Š	
	MOTA	2635	Ō	нон	34		711		114.948	1.00	8.16	š	
	MOTA	2636	0	нон	35		658	6.477	79.773	1.00		s	
	MOTA	2637	0	нон	36		262	7.930	95.115	1.00		s	
45	ATOM	2638	٥	HOH	38		341	-0.450	103.081	1.00	3.96	Š	
	MOTA	2639	0	нон	40	20.	527	12.061	101.135	1.00		s	
	MOTA	2640	Ο.	нон	42	31.	548	4.510	82.184	·1.00	13.63	s	
	MOTA	2641	0	нон	44	20.	139	3.415	109.317	1.00	9.63	S	
	ATOM	2642	0 .	HOH	46	38.	748		117.615	1.00		s	
50	MOTA	2643	0	нон	48	37.	332	6.832	98.871	1.00	20.54	S	
	MOTA	2644	0	нон	50	15.	243	1.107	105.237	1.00	7.71	S	
	MOTA	2645	0	нон	52	23.	362	13.594	103.308	1.00	16.03	s	
	MOTA	2646	0	HOH	54	24.	373	1.678	79.508	1.00	21.19	S	
	MOTA	2647	0	нон	55	38.	272	4.890	80.366	1.00	15.34	s	
55	MOTA	2648	0	нон	60	28.	231	24.639	95.411	1.00	10.59	s	
	MOTA	2649	0	нон	61	39.	120	8.121	96.836	1.00	17.30	S	
	ATOM	2650	0	нон	63	18.	805	15.804	105.109	1.00	24.81	S	
	MOTA	2651	0	нон	64	40.	943	11.048	89.550	1.00	24.53	S.	
~ 0	MOTA	2652	0	нон	68	31.	035	20.952	88.723	1.00	17.53	s	
60	MOTA	2653	0	нон	69	19.	610	-3.671	118.241	1.00	28.77	s	
	MOTA	2654	0	нон	70	23.	256	19.519	117.749	1.00	12.03	s	
	ATOM	2655	0	нон	71	21.	279	14.920	97.265	1.00	17.07	s	
	ATOM	2656	0	нон	72		571	8.465	98.099	1.00	17.54	S	
	ATOM	2657	0	нон	73		219	-7.157	96.638	1.00		s	
65	ATOM	2658	0	нон	74	14.	061		107.352	1.00		s	
	ATOM	2659	0	нон	75		428	6.714	101.400	1.00	20.61	S	
	MOTA	2660	0	нон	76		147	6.297	79.763	1.00	6.93	S	
	ATOM	2661	0	нон	78				110.664	1.00	42.69	s	
70	MOTA	2662	0	нон	79		740	11.793	96.499	1.00	19.31	S	
70	MOTA	2663	0	нон	82		334		104.252	1.00	25.92	S	
	MOTA	2664	0	нон	83		296	4.768	77.136	1.00	31.56	s	
	MOTA	2665	Ο.	нон	84		800	16.450	94.704	1.00	5.75	S	
	ATOM	2666	0	нон	87	45.	629	7.251	110.783	1.00	17.29	s	

	MOTA	2667	0	нон	90	13.592	18.093 -92	2.309	1.00 1	3 66	s	
	ATOM	2668	Ö	нон	91	9.122		5.091	1.00 3		S	
	ATOM	2669	ō	нон	92	16.369	12.885 106		1.00 2		Š	
-	MOTA	2670	0	HOH	93	13.386	21.050 89	9.915	1.00 1	7.97	S	
5	ATOM	2671	0	нон	94	11.913		.952	1.00 2		S	
	MOTA	2672	0	нон	95	20.093		9.951	1.00 1		· S	
	MOTA MOTA	2673 2674	0	нон Нон	96 97	17.551 20.767		7.296 1.877	1.00 2		S S	
	MOTA	2675	ŏ	нон	99	35.477		7.785	1.00 1		S	
10	ATOM	2676	ŏ	нон	101	21.955	8.778 118		1.00 2		s	
	ATOM	2677	ŏ	нон	102	40.041		1.678	1.00 1		S	
	MOTA	2678	0	нон	104	36.377	-3.662 102	2.275	1.00 1	8.75	S	
	MOTA	2679	0	HOH	106	3.852	11.665 120		1.00 3		S	
15	MOTA	2680	-	нон	108	39.673		.200	1.00 4		S	
13	MOTA	2681	0	HOH	110	6.144		2.235	1.00 5		S	
	MOTA MOTA	2682 2683	0	нон нон	111 112	30.628 30.065		2.526	1.00 2		S	
	MOTA	2684	ő	нон	113	14.004	8.985 104		1.00 2		S	
	ATOM	2685	ŏ	нон	114	33.791		.652	1.00 1		S	
20	MOTA	2686	0	HOH	117	22.111	19.027 120	746	1.00 3		S	
	MOTA	2687	0	HOH	118	26.607		.656	1.00 1	7.38	S	
	MOTA.	2688	0	нон	121	21.035	-9.445 110				S	
	ATOM	2689	0	нон	122	32.184	14.826 101		1.00 1		s	
25	MOTA MOTA	2690 2691	0	нон	123 124	17.599 34.130	-1.616 90 25.646 110).813	1.00 1		s s	
	MOTA	2692	ŏ	нон	126	9.990		3.389	1.00 1		. S	
	ATOM	2693	ŏ	нон	129	3.202		.601	1.00 5		s	
	MOTA	2694	0	нон	130	13.955	10.696 95	.694	1.00 1	9.43	s	
20	MOTA	2695	0	нон	131	31.703		3.664	1.00 2		s	
30	MOTA	2696	0	нон	132	35.057		.606	1.00 40		s	
	ATOM	2697 - 2698	0	нон	134	15.475		6.631	1.00 1		S	
	ATOM ATOM	· 2698 2699	0	нон Нон	135 136	17.594 7.395	16.623 102 -14.251 99	0.064	1.00 2		s s	
	ATOM	2700	ŏ	нон	137	16.245	22.597 107		1.00 1		S	
35	ATOM	2701	ŏ	нон	139	9.431		.038	1.00 3		Š	
	MOTA	2702	0	HOH	145	19.183		.555	1.00 4		s	
	MOTA	2703	0	нон	146	27.383	12.738 122		1.00 2	2.34	S	
	ATOM	2704	0	нон	148	39.078		.184	1.00 3		S	
40	MOTA	2705	0	нон	149	49.726		5.574	1.00 43		s	
40	MOTA MOTA	2706 2707	0	нон Нон	151 152	13.531 49.848	20.213 113 18.275 102		1.00 3		s s	
	ATOM	2708	ŏ	нон	153	27.728	-14.666 103		1.00 3		S	
	ATOM	2709	ō	нон	154	17.610		.633		2.29	s	
4-	MOTA	2710	0	нон	155	16,723	19.937 85	.776	1.00 24	4.59	s	
45	MOTA	2711	0	нон	158	31.015		821		1.57	S	
	MOTA	2712	0	нон	159	39.461	15.014 103		1.00 3		s	
	MOTA MOTA	2713 2714	0	нон Нон	164 166	45.236 28.893	2.614 116 5.418 123			3.66 0.64	s s	
	ATOM	2715	ō	нон	167	35.887		.622		1.12	S	
50	ATOM	2716	ō	нон	168	29.323	-10.874 107			9.92	š	
	MOTA	2717	0	HOH	170	33.078	22.456 122		1.00 2		S	
	MOTA	2718	0	нон	171	6.377		.461		9.35	S	
	MOTA	2719	0	нон	175	38.059	24.742 100		1.00 44		s	
55	MOTA MOTA	2720 2721	0	нон нон	179 184	12.119 35.206	-0.723 109 -9.022 104		1.00 20	8.60	S S	
J J	MOTA	2722	ŏ	HOH ·		5.690		1.872	1.00 2		· S	
	ATOM	2723	ŏ	нон	187	3.662	-13.329 100	.868	1.00 2		s	
	MOTA	2724	0	нон	188	8.547		. 499	1.00 3		s	
<i>(</i> 0	MOTA	2725	0	нон	189	13.396	13.012 123		1.00 2		s	
60	MOTA	2726	0	нон	190	37.857		.808	1.00 1		S	
	MOTA	2727	0	нон	191	15.390		.556	1.00 3		S	
	MOTA MOTA	2728 2729	0	нон нон	192 195	24.877 7.560		.150	1.00 3		s s	
	ATOM	2730	ŏ	нон	197	38.275	1.921 103 6.762 75	.942	1.00 2		. S	
65	ATOM	2731	ŏ	нон	198	11.981	14.135 109		1.00 20		S	
	ATOM	2732	ŏ	нон	199			.699	1.00 3		s	
	ATOM	2733	0	нон	201		-10.638 103		1.00 3		Š	
	ATOM .	2734	0	нон	203	25.859		.393	1.00 3		S	
70	MOTA	2735	0	нон	205			647	1.00 1		S	
70	MOTA MOTA	2736 2737	0	нон нон	207 208	23.255 7.965		.372	1.00 28		S	
	MOTA	2738	Ö	нон	210			.337	1.00 3		S S	
	MOTA	2739	ŏ	нон	211	23.200	15.157 105			3.65	s	

	ATOM MOTA	2740 2741	0	нон	212 215	16.820 37.029	11.748	98.364 102.172	1.00 4.40 1.00 9.34	S
	ATOM	2742	ŏ	нон	217	45.218	10.237	90.158	1.00 50.32	S
	ATOM	2743	ŏ	нон	220	46.617		108.402	1.00 29.26	š
5	ATOM	2744	ō	нон	221	18.955	8.984	95.378	1.00 23.41	Š
	ATOM	2745	0	нон	223	22.905		118.403	1.00 15.81	S
	ATOM	2746	0	нон	225	2.959	-6.265	97.196	1.00 46.93	s
•	MOTA	2747	0	нон	226	11.436		109.490	1.00 15.86	S
10	ATOM	2748	0	нон	228	16.698		102.916	1.00 25.42	S
10	ATOM	2749	0	нон	229	14.674		106.079	1.00 26.44	S
	ATOM ATOM	2750	.0	нон	232	21.595	-5.809	87.827	1.00 14.15	S
	MOTA	2751 2752	0	нон	233 238	11.151		115.185	1.00 32.57	S
	ATOM	2753	Ö	нон	241	29.371 13.508	-3.075 12.891	77.740 99.625	1.00 19.94 1.00 20.34	s s
15	MOTA	2754	ŏ	нон	243	17.423		118.567	1.00 24.32	S
	MOTA	2755	ō	нон	244	21.246	6.736	82.924	1.00 39.07	š
	ATOM	2756	ō	нон	245	11.590	19.689	98.284	1.00 19.24	Š
	ATOM	2757	ō	нон	247	51.802		117.095	1.00 55.38	Š
	ATOM	2758	0	нон	251	8.180	5.024	99.128	1.00 31.61	S
20	MOTA	2759	0	HOH	252	21.300	12.368	98.575	1.00 31.29	s
	MOTA	2760	0	нон	253	41.894	8.695	97.607	1.00 30.47	S
	ATOM	2761	0	нон	254	23.625		121.375	1.00 27.92	s,
	MOTA	2762	0	нон	255	29.438		123.667	1.00 26.17	S
25	ATOM	2763	ŏ	HOH	256	20.446		116.657	1.00 34.15	·S
25	ATOM ATOM	2764 2765	0	нон Нон	257 260	11.975 13.789	9.878	91.516 113.975	1.00 18.84 1.00 23.75	s s
	ATOM	2766	ŏ	нон	262	7.623		124.008	1.00 30.74	S.
	ATOM	2767	ŏ	нон	263	20.395	4.227	81.694	1.00 33.87	Ş
	ATOM	2768	ō	нон	266	34.255	-0.467	81.343	1.00 30.08	Š
30	MOTA	2769	Ó	HOH	268	45.417		105.917	1.00 33.79	s
	ATOM	2770	0	нон	271	15.540	-18.971	104.185	1.00 36.81	S
	MOTA	2771	0	нон	272	31.560	28.306	95.365	1.00 25.41	Ş
	MOTA	2772	0	нон	273	10.820		124.773	1.00 27.96	S
35 ·	MOTA	2773	0	нон	275	16.259		106.228	1.00 15.83	S
33	MOTA	2774	0	нон	279	14.255		104.198	1.00 21.24	S
•	ATOM ATOM	2775 2776	0	нон	280 281	14.152 28.645	-13.914	109.944	1.00 30.26 1.00 35.08	s s
	ATOM	2777	ŏ	нон	283	15.855	18.951		1.00 35.08	S
	MOTA	2778	ŏ	нон	288	15.557		116.261	1.00 19.13	S
40	MOTA	2779	ŏ	нон	290	52.550	19.096	99.218	1.00 47.57	S
	ATOM	2780	Ō	нон	291	26.202	14.680	81.794	1.00 53.97	Š
	ATOM	2781	0	нон	294	20.086	20.598	120.312	1.00 37.20	S
	MOTA	2782	0	нон	295	6.012	19.892	120.875	1.00 18.20	s
45	ATOM	2783	0	нон	296	30.916		103.939	1.00 37.71	S
43	ATOM	2784	0	нон	.297	46.048		120.452	1.00 43.25	S
	ATOM ATOM	2785 2786	0.	нон	299	31.569		101.042	1.00 32.15	S
	MOTA	2787	0	нон	300 303	21.162 9.761	-3.401	87.125 112.502	1.00 32.61 1.00 27.58	s s
	MOTA	2788	ŏ	нон	305	32.066		112.302	1.00 27.38	5 5
50	ATOM	2789	ŏ	нон	307	33.480	-2.576	83.015	1.00 27.49	S
	MOTA	2790	o	нон	308	2.984		120.708	1.00 31.57	s
	MOTA	2791	0	нон	309	34.596	-15,790	94.772	1.00 43.06	. S
	ATOM	2792	0	нон	310	34.476		104.147	1.00 46.76	s
55	ATOM	2793	0	нон	313	18.109	-9.045	87.036	1.00 25.07	s
22	MOTA	2794	0	нон	314	2.837		121.659	1.00 42.28	S
	MOTA	2795	0	нон	315	13.698		111.141	1.00 35.74	S
	ATOM ATOM	2796 2797	0	НОН	317		18.005 -3.283		1.00 28.52	S
	MOTA	2798	0	нон нон	318 319	29.111 32.667		83.701 105.431	1.00 38.21 1.00 27.32	S. S
60	MOTA	2799	ŏ	нон	323		-19.468	88.447	1.00 27.32	S
	ATOM	2800	ō	нон	324	-2.283	-4.890	97.004	1.00 48.36	s
	ATOM	2801	ō	нон	327	28.636		118.234	1.00 30.32	ş
	MOTA	2802	0	нон	328	29.441		120.010	1.00 30.29	Š
	MOTA	2803	0	нон	331	25.024	1.315	88.662	1.00 35.16	S
65	MOTA	2804	0	нон	332	25.076	33.728	92.315	1.00 37.36	S
	MOTA	2805	0	нон	334	17.967	17.125	84.628	1.00 44.99	S
	MOTA	2806	0	нон	336	35.277	-4.775	82.255	1.00 22.90	S
	MOTA	2807	0	нон	338	5.655	-0.231	95.494	1.00 39.33	S
70	ATOM	2808	0	нон	340	46.414		108.144	1.00 58.72	S
,,	ATOM ATOM	2809 2810	0	нон нон	342 344	10.262 48.378	-2.840	88.835 102.187	1.00 36.82	s s
	ATOM	2811	ŏ		345	7.840		118.967	1.00 54.06	S
	ATOM	2812	Ō.	нон		42.036	-0.811	90.785	1.00 34.08	S

	MOTA	2813	٥	нон	351	51.775	6.542	133.541	1.00 37.45	s
	ATOM	2814	0	нон	354	31.545	13.101	. 83.668	1.00 37.78	S
	MOTA	2815	O	HOH	355	35.526	14.686	100.364	1.00 8.84	S
_	MOTA	2816	0	нон	361	12.290	20.796	107.012	1.00 17.59	S
5	MOTA	2817	0	HOH	363	40.627	4.272	127.391	1.00 41.84	S
	ATOM	2818	0	HOH	365	30.371	-1.879	79.833	1.00 13.67	S
	ATOM	2819	0	HOH	367	11.687	18.291	107.264	1.00 22.06	S
	ATOM	2820	٥	HOH	370	18.511	7.004	119.773	1.00 38.47	S
	MOTA	2821	0	HOH	371	17.908	- 13.463	100.054	1.00 12.12	s
10	MOTA	2822	0	HOH	372	27.131	-3.005	76.310	1.00 16.74	S
	MOTA	2823	٥	HOH	375	8.972	7.528	97.923	1.00 26.11	· s
	MOTA	2824	0	HOH	377	18.727	10.788	84.519	1.00 41.33	S
	MOTA	2825	0	HOH	379	14.127	15.750	98.863	1.00 25.29	S
	MOTA	2826	0	нон	383	41.700	9.858	81.807	1.00 33.52	S
15	MOTA	2827	0	HOH	385	35.261	15.280	106.016	1.00 28.87	S
	MOTA	2828	0	HOH	386	12.726		115.689	1.00 46.81	s
	ATOM	2829	. 0	HOH	393	43.648	7.839	106.741	1.00 16.47	· s
•	MOTA	2830	0	HOH	394	37.259		104.054	1.00 14.17	S
20	ATOM	2831	0	нон	396	24.282	-6.502	87.829	1.00 42.62	S
20	MOTA	2832	0	нон	400	43.027	-3.036	92.095	1.00 34.87	S
	MOTA	2833	0	нон	406	. 31.066	-3.244	81.803	1.00 24.95	S
	MOTA	2834	0	HOH	409	36.251		119.019	1.00 19.28	s
	MOTA	2835	0	HOH	415	10.534		100.073	1.00 39.35	S
25	ATOM	2836	0	нон	418	8.054		110.289	1.00 45.64	S
25	MOTA	2837	0	нон	422	39.306		111.576	1.00 34.28	· s
	MOTA	2838	0	нон	425	6.396		103.157	1.00 32.56	S
	MOTA	2839	0	нон	426	39.952	24.546	98.144	1.00 27.08	s
	MOTA	2840	0	нон	429	39.863	6.685	82.133	1.00 40.09	s
30	MOTA	2841	0	нон	430	21.921	12.487	85.799	1.00 40.68	S
3 0	MOTA	2842	0	нон	433	11.505		100.809	1.00 30.56	S
	MOTA	2843	0	нон	435	10.302		104.901	1.00 29.96	S
	MOTA	2844	0	нон	438	23.476	-0.876	78.128	1.00 28.68	S
	MOTA	2845	0	нон	442.			100.914	1.00 39.98	S
35	MOTA MOTA	2846 2847	0	нон	444 445	36.147 23.713	28.207	94.921 119.077	1.00 46.43	s
JJ	ATOM	2848	0	НОН	447	27.306	-4.631	90.698	1.00 42.21	S
	MOTA	2849	0	нон	448	45.805		107.875	1.00 43.77	s
	MOTA	2850	Ö	нон	449	11.162		125.577	1.00 28.04	S S
	MOTA	2851	ŏ	нон	450	51.897		132.993	1.00 42.08 1.00 37.33	5
40	MOTA	2852	Ö	нон	452	28.491		119.002	1.00 37.33	s s
-10	MOTA	2853	ŏ	нон	454	8.173		105.141	1.00 50.50	S
	ATOM	2854	ő	нон	459	42.750	5.736	87.519	1.00 36.93	S
	MOTA	2855	ö	нон	460	30.376	34.460	94.131		
	ATOM	2856	0	нон	466	25.986		120.060	1.00 31.43 1.00 52.81	s s
45	MOTA	2857	ŏ	нон	467	22.489		108.669	1.00 32.81	S
,,,	ATOM	2858	ŏ	нон	468		-2.077	86.180	1.00 23.27	S
	END	2070	v	non	400 .	23.302	-2.077	30.180	1.00 37.76	3
	س م									

TABLE 2

	REMARK	1	Сощо	ound	1-7_3d	pb.pdb mo	lecule	В			
_	CRYST		.250				90.00	90.	00 90.00	P212121	
5	MOTA	20	CB	LYS	17	24.3	52 -12.	458	60.280	1.00 51.00	В
	MOTA	21	CG	LYS	17	22.8	74 -12.	492	59.882	1.00 53.34	В
	MOTA	22	CD	LYS	17	22.6	63 -12.	316	58.375	1.00 53.77	В
	MOTA	23	CE	LYS	17	23.1	97 -13.	512	57.582	1.00 54.85	В
10	ATOM	24	.NZ	LYS	17	24.6	82 -13.	693	57.700	1.00 53:86	В
10	MOTA	25	С	LYS	17		06 -10.		59.443	1.00 47.83	В
	MOTA	26	0	LYS	17		75 -10.		58.419	1.00 48.69	В
	ATOM	27	N	LYS	17		45 -10.		61.888	1.00 49.93	В
	ATOM	28	CA	LYS	17		11 -11.		60.601	1.00 49.15	В
15	MOTA	29	N	ASN	18	23.5		260	59.599	1.00 45.98	В
13	ATOM	30	CA	ASN	18	23.2		340	58.535	1.00 43.66	В
	MOTA	31	CB	ASN	18	21.9		627	58.880	1.00 45.49	В
	MOTA MOTA	32 33	CG	asn Asn	18 18	20.74 20.4		481	58.599 57.442	1.00 49.80	9 B
	ATOM	34		ASN	18	20.0		856	59.653	1.00 50.22	. В
20	ATOM	35	C	ASN	18	24.3		336	58.180	1.00 41.30	В
	ATOM	36	ŏ	ASN	18	24.6		173	57.006	1.00 41.62	₿.
	ATOM	37	N	ILE	19	24.90		669	59.179	1.00 37.77	·B
	ATOM	38	CA	ILE	19	25.94		679	58.928	1.00 34.25	В
	MOTA	39	СВ	ILE	19	26.32		966	60.253	1.00 35.25	В
25	MOTA	40	CG2	ILE	19	26.54	48 -5.	988	61.346	1.00 38.29	В
	MOTA	41	CG1	ILE	19	27.58	B1 -4.	139	60.078	1.00 35.22	В
	ATOM	42	CD1	ILE	19	28.04		487	61.347	1.00 36.16	В
	MOTA	43	С	ILE	19	27.2		272	58.266	1.00 31.28	В
20	MOTA	44	0	ILE	19	27.7		287	58.722	1.00 31.52	В
30	MOTA	45	N	GLN	20	27.69		639	57.194	1.00 27.50	В
	MOTA	46	CA	GLN	20	28.90		091	56.483	1.00 26.14	В
	MOTA	47	CB	GLN	20	28.88		603	54.996	1.00 25.10	В
	MOTA	48	CG	GLN	20	30.27		495	54.347	1.00 27.01	В
35	MOTA MOTA	49 50	CD	GLN GLN	20 20	30.23 29.92		169 026	52.843 52.016	1.00 29.81	В
55	ATOM	51		GLN	20	30.5		924	52.493	1.00 30.67	B B
	MOTA	52	C	GLN	20	30.16		567	57.176	1.00 30.62	В
	ATOM	53	ō	.GLN	20	30.21		398	57.561	1.00 27.09	В
	ATOM	54	N	VAL	21	31.17		426	57.327	1.00 22.08	В
40	MOTA	55	CA	VAL	21	32.42		048	57.989	1.00 18.37	В
	MOTA	56	CB	VAL	21	32.47		584	59.471	1.00 19.87	В
	MOTA	57	CG1	VAL	21	33.80	02 -6.	230	60.125	1.00 16.85	В
	MOTA	58	CG2	VAL	21	31.30	00 -6.	004	60.291	1.00 14.97	В
15	MOTA	59	С	VAL	21	33.64		567	57.221	1.00 18.19	В
45	MOTA	60	Ο.	VAL	21	33.84		771	57.081	1.00 16.60	В
	ATOM	61	N	VAL	22	34.45		637	56.722	1.00 17.58	В
	MOTA	62	CA:	VAL	22	35.65		965	55.967	1.00 15.68	В
	MOTA MOTA	63 64	CB	VAL VAL	· 22	35.56		385	54.532	1.00 17.56	В
50	ATOM	65		VAL	22	34.30 35.59		889 863	53.846 54.575	1.00 17.79	B B
50	ATOM	66	C	VAL	22	36.86		396	56.693	1.00 17.41	. В
	ATOM	67	ŏ	VAL	22	36.74		502	57.549	1.00 14.89	В
	ATOM	68	N	VAL	23	38.03		936	56.358	1.00 14.83	B
	ATOM	69	CA	VAL	23	39.30		534	56.972	1.00 13.82	B
55	ATOM	70	CB	VAL	23	39.93		745	57.768	1.00 13.54	В
	MOTA	71		VAL	23	41.33	30 -6.	405	58.282	1.00 6.83	В.
	MOTA	72	CG2	VAL	23	39.03	34 -7.	112	58.944	1.00 13.12	В
	MOTA	73	С	VAL	23	40.30		023	55.928	1.00 13.37	В
۷۸	MOTA	74	0	VAL	23	40.41		576	54.835	1.00 10.49	В
60	MOTA	75	N	ARG	24	41.00		944	56.256	1.00 14.76	В
	ATOM	76	CA	ARG	24	42.01		407	55.346	1.00 17.25	В
	MOTA	77	CB	ARG	24	41.57		087	54.700	1.00 14.29	В
	ATOM	78	CG	ARG	24	42.52		660	53.590	1.00 12.98	В
65	MOTA	79	CD	ARG	24	42.33		225	53.130	1.00 9.77	В
U)	MOTA	80	NE CZ	ARG	24	42.97		006	51.838	1.00 9.97	В
	ATOM ATOM	81 82	CZ NH1	ARG ARG	24 24	42.88 42.16		111 143	51.112 51.544	1.00 9.72	В
	MOTA	83	NH2		24	43.47		177	49.923	1.00 3.96 1.00 8.75	B B
	ATOM	84	C	ARG	24	43.32		180	56.098	1.00 18.12	В
70	ATOM	85	ŏ	ARG	24	43.38		408	57.055	1.00 16.79	В
-	ATOM	86	N	CYS	25	44.37		874	55.657	1.00 21.17	В
									•	. = :	=

•	MOTA	87	CA	CYS	25	45.688	-3.764	56.268	1.00 23.23	В
	MOTA	88	CB	CYS	25	46.415	-5.140	56.254	1.00 23.67	В
	MOTA	89	SG	CYS	25	48.096	-5.149	56.970	1.00 28.58	. В
_	MOTA	90	C	CYS	25	46.464	-2.764	55.443	1.00 24.61	В
5	MOTA	91		CYS	25	46.457	-2.836	54.211	1.00 24.46	В
	MOTA	92	N ·	ARG	26	47.116	-1.818	56.109	1.00 25.36	В
	MOTA	93		ARG	26	47.897	-0.829	55.380	1.00 27.69	В
	ATOM	94		ARG	26	48.087	0.458	56.219	1.00 26.88	В
	ATOM	95		ARG	26	49.165		57.300	1.00 25.37	В
10	ATOM	96		ARG	26	49.817	1.722	57.544	1.00 26.81	В
	ATOM	97		ARG	26	51.181	1.599	58.060	1.00 30.34	. B
	MOTA	98		ARG	26	51.504	1.598	59.349	1.00 31.91	В
	MOTA	99	NH1		26	50.566	1.721	60.277	1.00 32.84	В
	ATOM	100	NH2		26	52.767	1.459	59.714	1.00 33.10	В
15	MOTA	101		ARG	26 .	49.268	-1.423	55.072	1.00 29.73	В
	ATOM	102		ARG	26	49.673	-2.417	55.676	1.00 28.95	В
	ATOM	103		PRO	27	49.991	-0.832	54.108	1.00 31.27	·B
	ATOM	104		PRO	27	49.498	0.108	53.083	1.00 32.66	В
	ATOM	105		PRO	27	51.327	-1.324	53.757	1.00 32.62	В
20	ATOM	106		PRO	27	51.452	-0.937	52.287	1.00 31.65	В
	MOTA	107		PRO	27	50.745	0.369	52.235	1.00 31.82	В
	ATOM	108		PRO	27	52.372	-0.626	54.642	1.00 33.24	В
	ATOM	109		PRO	27	52.065	0.364	55.311	1.00 33.24	В
	ATOM	110		PHE	28	53.599	-1.141	54.652	1.00 34.79	В
25	MOTA	111		PHE	28	54.670	-0.545	55.451	1.00 34.79	- B
23	MOTA	112		PHE	28	55.890	-1.393	55.401	1.00 34.86	
	ATOM	113		PHE	28	55.756	-2.691	56.124	1.00 33.35	. B B
	ATOM	114	CD1		28	55.856	-3.893	55.440	1.00 33.06	В
	MOTA	115	CD2		28	55.590	-2.715	57.507	1.00 31.83	B
30	ATOM	116	CE1		28	55.801	-5.102	56.128		
50	ATOM	117	CE2		28				1.00 31.40.	В.
						55.536	-3.918	58.193	1.00 30.69	В
	MOTA MOTA	118 119		PHE	28 28.	55.644	-5.112	57.500 54.956	1.00 29.86 1.00 36.62	В
		120		PHE		55.043	0.842			В
35	MOTA			PHE ASN	28	55.102	1.080	53.752	1.00 36.72	В
55	ATOM	121 122		ASN	29 29	55.297 55.687	1.755 3.109	55.885 55.517	1.00 39.15	В
	MOTA			ASN					1.00 43.00	В
•	MOTA	123			29	55.449	4.078	56.693	1.00 41.82	В
	ATOM	124		ASN	29 29	55.787	3.460	58.044	1.00 41.11	В
40	MOTA	125	OD1			56.953	3.237	58.367	1.00 38.49	В
70	MOTA	126	ND2		29	54.758	3.178	58.838	1.00 40.06	B
	MOTA	127		ASN	29	57.160	3.083	55.130	1.00 46.95	В
	MOTA	128		ASN	29	57.913	2.236	55.621	1.00 48.65	В
	MOTA	129		LEU	30	57.554	3.998	54.243	1.00 49.22	В
45	MOTA	130		LEU	30	58.930	4.106	53.751	1.00 49.70	В
73	MOTA	131		LEU	30	59.142	5.490	53.121	1.00 49.24	В
	MOTA	132 133		LEU	. 30	60.429	5.757	52.341	1.00 49.29	В
	MOTA		CD1		30	60.294	7.104	51.640	1.00 49.07	В
	MOTA	134	CD2		30	61.643	5.740	53.264	1.00 49.24	В
50	MOTA MOTA	135 136		LEU	30	59.989	3.866	54.823	1.00 51.07	В
50				LEU	30	60.877	3.032	54.649	1.00 50.68	В
	MOTA	137 138		ALA	31	59.889	4.605	55.925	1.00 52.87	В
	MOTA	. 139		ALA	31	60.831	4.497	57.035	1.00 54.80	В
	MOTA MOTA			ALA	31	60.399	5.420	58.157	1.00 53.50	В
55		140		ALA	31	61.011	3.077	57.576	1.00 56.55	В
55	MOTA	141		ALA	31	62.140	2.649	57.837	1.00 56.62	В
	ATOM	142		GLU	32	59.906	2.354	57.751	1.00 59.00	В
	MOTA	143		GLU	32	59.958	0.989	58.272	1.00 61.92	В
	ATOM	144		GLU	32	58.625	0.631	58.999	1.00 61.49	В
60	MOTA	145		GLU	32	57.413	0.441	58.094	1.00 60.80	В
UU	MOTA	146		GLU	32	56.101	0.376	58.872	1.00 59.87	В
	MOTA	147	OE1		32	55.038	0.196	58.242	1.00 58.45	В
	MOTA	148	OE2		32	56.129	0.514	60.115	1.00 60.23	В
	MOTA	149		GLU	32	60.270	-0.057	57.198	1.00 64.49	В.
65	MOTA	150		GLU	32	60.610	-1.199	57.522	1.00 64.33	. В
03	MOTA	151		ARG	33	60.148	0.330	55.927	1.00 67.16	В
	MOTA	152		ARG	33	60.447	-0.573	54.813	1.00 69.70	В
	MOTA	153		ARG	33	59.996	0.033	53.435	1.00 71.95	В
	MOTA	154		ARG	33	58.567	0.570	53.353	1.00 75.31	В
70	MOTA	155		ARG	33	58.383	1.377	52.056	1.00 78.38	В
70	ATOM	156		ARG	33	57.203	2.248	52.066	1.00 80.30	В
	MOTA	157		ARG	33	56.937	3.167	51.136	1.00 80.67	В
	ATOM	158	NH1		33	57.766	3.345	50.114	1.00 79.70	. В
	MOTA	159	NH2	ARG	33	55.841	3.913	51.226	1.00 80.30	В

	MOTA	160	С	ARG	33	61.965	-0.720	54.794	1.00 70.18	В
	ATOM	161	0	ARG	33	62.502	-1.813	54.599	1.00 70.13	В
	MOTA	162	N	LYS	34	62.638	0.411	54,997	1.00 70.20	· в
_	MOTA	163	CA	LYS	34	64.094	0.483	55.012	1.00 70.34	В
5		164	CB	LYS	34	64.552	1.980	55.063	1.00 71.26	В
	MOTA	165	CG	LYS	34	66.041	2.209	54.795	1.00 71.67	В
	MOTA	166	CD	LYS	34	66.407	3.688	54.868	1.00 71.50	В
	MOTA	167	CE	LYS	34 34	66.116	4.260	56.251	1.00 72.55 1.00 72.95	B B
10	ATOM ATOM	168 169	NZ C	LYS LYS	34	66.513 64.644	5.694 -0.288	56.388 56.211	1.00 72.95	B
10	MOTA	170	ò	LYS	34	65.707	-0.915	56.123	1.00 70.68	В
	MOTA	171	N	ALA	35	63.921	-0.236	57.330	1.00 68.80	В
	MOTA	172	CA	ALA	35	64.324	-0.952	58.540	1.00 67.64	В
	ATOM	173	CB	ALA	35	63.605	-0.381	59.760	1.00 67.24	В
15	MOTA	174	С	ALA	35	63.958	-2.424	58.356	1.00 66.54	В
	MOTA	175	0	ALA	35 ·	64.075	-3.232	59.286	1.00 65.43	В
	MOTA	176	N	SER	36	63.520	-2.750	57.138	1.00 64.95	В
	MOTA	177	CA	SER	36	63.113	-4.099	56.770	1.00 63.77	В
20	MOTA	178	CB	SER	36	64.347	-4.974	56.532	1.00 63.33	В
20	MOTA	179	og	SER	36 36	65.136	-4.438 -4.670	55.481	1.00 61.84	. В
	MOTA MOTA	180 181	C	SER SER	36 36	62.240 62.731	-5.313	57.879 58.810	1.00 63.32 1.00 63.79	B
	ATOM	182	N	ALA	37	60.939	-4.417	57.772	1.00 61.85	В.
	MOTA	183	CA	ALA	37	59.989	-4.873	58.773	1.00 59.96	B
25	MOTA	184	СВ	ALA	37	58.921	-3.806	58.987	1.00 59.90	В
	MOTA	185	С	ALA	37	59.344	-6.219	58.442	1.00 58.87	В
	MOTA	186	0	ALA	37	58.975	~6.499	57.301	1.00 58.65	В
	ATOM	187	N	HIS	38	59.215	-7.038	59.479	1.00 57.20	В
30	MOTA	188	CA	HIS	38	58.638	-8.378	59.411	1.00 54.48	В
30	MOTA	189	CB	HIS	38	59.315	-9.263	60.513	1.00 56.18	В
	MOTA	190	CG	HIS	38	59.436	-8.582	61.851	1.00 56.74	В
•	ATOM ATOM	191 192		HIS HIS	38 38	59.058 60.024	-8.977 -7.344	63.092 62.011	1.00 57.32 1.00 55.67	B B
	ATOM	193		HIS	38	60.005	-7:006	63.288	1.00 56.12	В
35 ·		194		HIS	38	59.424	-7.980	63.967	1.00 57.53	В
٠.	ATOM	195	C	HIS	38	57.118	-8.352	59.615	1.00 51.90	В
	ATOM	196	0	HIS	38	56.642	-8.343	60.754	1.00 52.05	В
	ATOM	197	N	SER	39	56.356	-8.350	58.523	1.00 47.82	В
40	MOTA	198	CA	SER	39	54.893	-8.320	58.619	1.00 44.47	В
40	ATOM	199	CB	SER	39	54.255	-8.336	57.219	1.00 43.58	В
	MOTA	200	OG	SER	39	52.837	-8.377	57.305	1.00 37.62	В
	MOTA	201	Ċ	SER	39	54.303	-9.468	59.435	1.00 43.06	В
	MOTA MOTA	202 203	O N	SER ILE	39 40	54.681 53.373	-10.624 -9.144	59.246 60.334	1.00 42.78	B B
45	MOTA	204	CA	ILE	40		-10.162	61.157	1.00 39.33	B
	ATOM	205	CB	ILE	40	52.660	-9.761	62.665	1.00 39.17	В
	MOTA	206		ILE	40 .	54.063	-9.542	63.215	1.00 38.53	В
	MOTA	207		ILE	40	51.824	-8.511	62.858	1.00 39.67	В
	MOTA	208	CD1	ILE	40	51.496	-8.238	64.319	1.00 38.82	В
50	MOTA	209	C	ILE	40		-10.456	60.663	1.00 38.28	В
	MOTA	210	0	ILE	40		-11.249	61.265	1.00 37.83	В
	MOTA	211	N	VAL	41	50.932	-9.837	59.550	1.00 38.34	. В
	MOTA MOTA	212 213	CA CB	VAL VAL	41 41		-10.047	59.000	1.00 38.90	В
55	MOTA	214		VAL	41	48.792 47.421	-8.724 -8.971	58.956 58.345	1.00 39.34	B B
<i></i>	MOTA	215		VAL	41	48.648	-8.154	60.360	1.00 38.41	В
	MOTA	216		VAL	41	49.535		57.612	1.00 38.55	В
	MOTA	217	Ó	VAL	41		-10.243	56.661	1.00 36.24	В.
	MOTA	218	N	GLU	42		-11.729	57.513	1.00 40.08	В
60	MOTA	219	CA	GLU	42		-12.433	56.255	1.00 42.70	В
	MOTA	220	CB	GLU	42		-13.916	56.393	1.00 45.52	В
	MOTA	221	CG	GLU	42		-14.215	56.163	1.00 47.68	В
	MOTA	222	CD	GLU	42		-15.636	56.578	1.00 50.75	В
65	MOTA MOTA	223 224		GLU	42		-16.576	56.323	1.00 52.01	В
55	MOTA	225	C	GLU	42 42		-15.816 -12.338	57.151 55.896	1.00 51.85 1.00 41.88	B B
	ATOM	226	0	GLU	42		-12.740	56.683	1.00 41.88	В
	ATOM	227	N	CYS	43		-11.798	54.718	1.00 40.93	В
	ATOM	228	CA	CYS	43		-11.670	54.275	1.00 41.17	В
70	MOTA	229	CB	CYS	43		-10.237	53.775	1.00 39.59	В
	ATOM	230	SG	CYS	43	44.959	-9.008	55.115	1.00 41.44	В
	ATOM	231	С.	CYS	43		-12.682	53.185	1.00 42.27	В
	MOTA	232	0	CYS	43	45.736	-12.781	52.182	1.00 43.23	В

										_
	MOTA	233	N	ASP	44		-13.435	53.394	1.00 43.10	В
	MOTA	234	CA	ASP	44		-14.444	52.436	1.00 43.06	В
	MOTA	235	CB	ASP	44		-15.831	53.138	1.00 45.99	В
5	MOTA	236	CG	ASP	44		-16.999	52.151	1.00 46.99	В
J	MOTA	237		ASP	44		-16.948	51.139	1.00 48.57	В
	ATOM .	238	OD2		44		-17.971	52.398	1.00 44.91	В
	MOTA	239	C	ASP	. 44		-14.045	51.853	1.00 42.13	В
	ATOM	240	0	ASP	44		-14.446	52.363	1.00 39.99	В
10	MOTA	241	N	PRO	45		-13.254	50.767 49.990	1.00 41.84	B B
10	MOTA	242	CD	PRO	45 45		-12.853		1.00 40.03	. B
	MOTA	243	CA CB	PRO PRO	45		-12.791	50.107 48.918	1.00 41.77	. В
	MOTA MOTA	244 245	CG	PRO	45		-12.001 -12.688	48.614	1.00 40.93	В
		245	C	PRO	45		-13.893	49.690	1.00 42.90	В
15	MOTA	247	Ö	PRO	45		-13.822	50.002	1.00 42.90	В
10	MOTA MOTA	248	N	VAL	46		-14.908	48.985	1.00 42.74	В
	ATOM	249	CA	VAL	46		-15.990	48.552	1.00 42.74	В
	MOTA	250	CB	VAL	46		-17.109	47.854	1.00 41.92	В
	MOTA	251	CG1		46		-18.269	47.531	1.00 40.40	В
20	MOTA	252	CG2		46		-16.574	46.581	1.00 41.19	В
	MOTA	253	c	VAL	46		-16.577	49.751	1.00 43.26	В
	ATOM ·	254	ŏ	VAL	46		-16.736	49.730	1.00 43.10	В
	ATOM	255	N	ARG	47		-16.896	50.797	1.00 43.54	В
	MOTA	256	CA	ARG	47		-17.455	52.007	1.00 44.21	В
25	ATOM	257	CB	ARG	47		-18.250	52.784	1.00 47.76	·B
	MOTA	258	CG	ARG	47		-19.635	52.203	1.00 52.08	. B
	MOTA	259	CD	ARG	47		-19.981	52.208	1.00 55.86	В
	ATOM	260	NE	ARG	47		-19.743	53.508	1.00 59.28	В
	ATOM	261	CZ	ARG	47		-20.346	54.638	1.00 60.15	В
30	MOTA	262	NH1		47		-21.237	54.639	1.00 60.50	В
-	MOTA	263	NH2		47		-20.051	55.770	1.00 60.66	В
	MOTA	264	c	ARG	47		-16.360	52.883	1.00 41.71	В
	ATOM	265	ŏ	ARG	47		-16.643	53.845	1.00 40.72	В
	ATOM	266	N	LYS	48		-15.112	52.537	1.00 39.92	В
35	MOTA	267	CA	LYS	48		-13.947	53.268	1.00 38.19	B
-	ATOM	268	СВ	LYS	48		-13.912	53.223	1.00 38.15	В
	ATOM	269	CG	LYS	48		-13.820	51.826	1.00 39.40	В
	ATOM	270	CD	LYS	48		-14.236	51.809	1.00 39.31	В
	ATOM	271	CE	LYS	48		-14.014	50.440	1.00 41.44	В
40	ATOM	272	NZ	LYS	48		-14.620	49.354	1.00 42.78	B
	ATOM	273	С	LYS	48		-13.925	54.723	1.00 37.09	В
	ATOM	274	ō	LYS	48		-13:563	55.617	1.00 37.31	В
	ATOM	275	N	GLU	49		-14.314	54.961	1.00 35.98	В
	MOTA	276	CA	GLU	49	40.450	-14.327	56.315	1.00 36.33	В
45	ATOM	277	CB	GLU	49	40.861	-15.733	56.743	1.00 40.35	В
	MOTA	278	CG	GLU	49	39.752	-16.767	56.761	1.00 46.19	В
	MOTA	279	CD	GLU	49	40.261	-18.163	57.122	1.00 49.22	В
	MOTA	280	OE1	GLU	49		-19.131	56.975	1.00 50.87	В
	MOTA	281	OE2	GLU	49	41.431	-18.293	57.555	1.00 49.58	В
50	ATOM	282	C	GLU	49	41.669	-13.444	56.445	1.00 35.96	В
	MOTA	283	0	GLU	49		-13.095	55.462	1.00 34.28	В
	MOTA	284	N	VAL	50		-13.097	57.685	1.00 34.47	В
	ATOM	285		VAL	50		-12.292	57.999	1.00 34.53	В
~ ~	MOTA	286	СВ	VAL	50		-10.858	58.439	1.00 32.83	В
55	ATOM	287	CG1		50		-10.918	59.512	1.00 30.31	В
	MOTA	288	CG2		50		-10.092	58.929	1.00 32.98	В
	MOTA	289	С	VAL	50		-13.059	59.135	1.00 35.60	В
	MOTA	290	0	VAL	50		-13.367	60.130	1.00 36.44	В
~	ATOM.	291	N	SER	51		-13.411	58.976	1.00 36.72	В
60	MOTA	292	CA	SER	51		-14.157	60.022	1.00 36.92	В
	ATOM	293	CB	SER	51		-15.481	59.447	1.00 37.59	В
	MOTA	294	OG	SER	51		-16.427	60.482	1.00 36.23	В
	ATOM	295	С	SER	51		-13.315	60.656	1.00 37.31	В
<i>C</i>	ATOM	296	0	SER	51		-12.731	59.960	1.00 36.32	· В
65	ATOM	297	N	VAL	52		-13.265	61.984	1.00 37.74	В
	ATOM	298	CA	VAL .			-12.474	62.735	1.00 39.56	В
	ATOM	299	CB	VAL	52		-11.558	63.749	1.00 38.44	В
	ATOM .	300	CG1		52		-10.668	64.454	1.00 37.83	В
70	MOTA	301	CG2		52		-10.737	63.042	1.00 37.78	В
70	MOTA	302	C	VAL	52		-13.328	63.507	1.00 41.45	В
	MOTA	303	0	VAL	52		-14.296	64.167	1.00 41.94	В
	ATOM	304	N	ARG	53		-12.968	63.434	1.00 43.18	В
	MOTA	305	CA	ARG	53	21.106	-13.713	64.166	1.00 46.04	В

	ATOM	306	CB	ARG	53	52 452	-13:698	63.434	1.00 45.91	В
	ATOM	307	CG	ARG	53	53.488	-14.619	64.064	1.00 44.72	В
	ATOM	308	CD	ARG	53	54.490	-15.103	63.034	1.00 45.80	В
	ATOM	309	NE	ARG	53		-14.018		1.00 46.75	
~								62.514		В
5	MOTA	310	CZ	ARG	53	56.036	-14.095	61.39B	1.00 45.30	В
	MOTA	311	NH1	ARG	53	56.028	-15.209	60.675	1.00 44.24	В
	MOTA	312		ARG	53		-13.056	61.011	1.00 44.19	В
	MOTA	313	С	ARG	53	51.259	-13.092	65.540	1.00 47.93	В
	MOTA	314	0	ARG	53	51 466	-11.884	65.667	1.00 48.40	В
1.0										
1.0	ATOM	315	N	THR	54	51.156	-13.929	66.565	1.00 49.62	В
	ATOM	316	·CA	THR	54	51.257	-13.473	67.941	1.00 51.39	В
	MOTA	317	CB	THR	54		-13.744	68.683		
									1.00 51.01	В
	ATOM	318	OGI	THR	54	49.735	-15.157	68.795	1.00 49.13	В
	ATOM	319	CG2	THR	54 .	48.775	-13.144	67.914	1.00 51.53	В
15	ATOM	320		THR	54					
13			С				-14.139	68.709	1.00 52.60	В
	ATOM	321	0	THR	54	52.439	-14.058	69.933	1.00 53.07	В
	ATOM	322	N	GLY	55	53 309	-14.784	67.995	1.00 54.10	В
	MOTA	323	CA	GLY	55		-15.459	68.666	1.00 57.08	В
	MOTA	324	С	GLY	55	55.721	-15.519	67.914	1.00 59.62	В
20	MOTA	325	0	GLY	55		-14.549	67.264	1.00 59.27	. В
	MOTA	326	N	GLY	. 56		-16.668	68.016	1.00 60.97	В
	ATOM	327	CA	GLY	56	57.682	-16.880	67.372	1.00 62.99	В
	ATOM	328	С	GLY	56		-16.549	65.892	1.00 64.76	
										В
05	ATOM	329	0	GLY	56	56.940	-15.828	65.350	1.00 66.18	· B
25	ATOM	330	N	LEU	57	58.818	-17.074	65.235	1.00 64.97	В
	ATOM	331	CA	LEU	57		-16.821	_		
								63.809	1.00 64.92	В
	ATOM	332	СВ	LEU	57	60.508	-17.137	63.407	1.00 63.43	В
	MOTA	333	CG	LEU	57 .	61.638	-16.508	64.258	1.00 63.25	В
	ATOM	334		LEU	57		-17.335		1.00 62.77	
30								65.520		В
30	MOTA	335	CD2	LEU	57	62.928	-16.452	63.459	1.00 61.76	В
	ATOM	336	С	LEU	57	58.080	-17.654	62.951	1.00 65.79	В
	MOTA	337	0	LEU	57		-18.328	63.470	1.00 65.88	В
	MOTA	338	N	ALA	58	58.269	-17.597	61.636	1.00 65.65	В .
	MOTA	339	CA	ALA	58	57 435	-18.356	60.712	1.00 65.12	В
35										
55	MOTA	- 340	СВ	ALA	58	57.687	-17.891	59.286	1.00 65.82	В
	ATOM	341	С	ALA	58	57.770	-19.838	60.847	1.00 64.20	В
	ATOM	342	0	ALA	58		-20.709	60.525	1.00 64.59	
										В
	MOTA	343	N	ASP	59		-20.099	61.340	1.00 62.61	В
	ATOM	344	CA	ASP	59	59.509	-21.447	61.542	1.00 60.18	В
40	ATOM	345	CB	ASP						
40					59		-21.335	62.035	1.00 60.66	В
	MOTA	346	CG	ASP	59	61.622	-22.682	62.266	1.00 61.45	В
	ATOM	347	OD1	ASP	59	61.396	-23.268	63.343	1.00 61.95	В
	ATOM	348		ASP	59					
							-23.155	61.370	1.00 61.61	В
	MOTA	349	С	ASP	59	58.663	-22.274	62.519	1.00 58.06	В
45	ATOM	350	0	ASP	59		-23.490	62.370	1.00 56.73	В
	MOTA	351	N	LYS	60		-21.591	63.513	1.00 55.07	В
	ATOM	352	CA	LYS	60	57.258	-22.200	64.528	1.00 52.63	В
	MOTA	353	CB	LYS	60		-23.079	65.525	1.00 51.66	В
50	MOTA	354	CG	LYS	60	57.301	-23.696	66.672	1.00 51.86	В
50	ATOM	355	CD	LYS	60	58.046	-24.839	67.368	1.00 51.88	В
	ATOM	356	CE	LYS	60		-24.373	68.011	1.00 53.18	В
	MOTA	357	NZ	LYS	60 .,	60.197	-25.492	68.528	1.00 52.09	В
	MOTA	358	С	LYS	60	56.615	-21.023	65.248	1.00 51.19	В
	MOTA	359	0	LYS	60		-20.124	65.724	1.00 51.41	В
55										
"	MOTA	360	N	SER	61		-21.010	65.313	1.00 48.55	В
	MOTA	361	CA	SER	61	54.599	-19.905	65.960	1.00 45.99	В
	MOTA	362	CB	SER	61		-18.636	65.192	1.00 46.32	В
										_
	MOTA	363	OG	SER	61	54.559	-18.803	63.820	1.00 44.99	В.
	ATOM	364	С	SER	61	53.092	-20.082	66.086	1.00 45.35	В
60 ·	MOTA	365	O	SER	61		-20.950			
-								65.449	1.00 44.81	В
	MOTA	366	N	SER	62	52.488	-19.242	66.922	1.00 43.72	В
	MOTA	367	CA	SER	62	51.047	-19.261	67.131	1.00 41.95	В
	ATOM	368	CB							
				SER	62		-19.050	68.592	1.00 41.39	В
	MOTA	369	OG	SER	62	51.608	-18.079	69.135	1.00 41.34	В
65	MOTA	370	С	SER	62		-18.143	66.291	1.00 40.85	В
	MOTA	371	0	SER	62		-17.229	65.872	1.00 39.19	В
	MOTA	372	N	ARG	63	49.138	-18.221	66.031	1.00 40.24	В
	ATOM	373	CA	ARG	63		-17.207	65.226	1.00 38.90	
										В
70	MOTA	374	CB	ARG	63		-17.514	63.695	1.00 39.76	В
70	ATOM	375	CG	ARG	63	50.074	-17.554	63.205	1.00 41.62	В
	ATOM	376	CD	ARG	63		-17.897			
								61.725	1.00 43.20	В
	ATOM	377	NE.	ARG	63	49.763	-16.776	60.866	1.00 46.47	В
	MOTA	378	CZ	ARG	63		-15.711	60.626	1.00 46.07	В
							,	30.020	,	

	MOTA	379	XIU1	ARG	63	51 770	-15.613	61.178	1.00 47.55	-
										В
	MOTA	380	NH2	ARG	63	50.090	-14.741	59.833	1.00 45.86	В
	ATOM	381	С	ARG	63	46.976	-17.131	65.558	1.00 37.75	В
	MOTA	382	ō	ARG	63		-18.050			
5								66.143	1.00 36.32	В
5	MOTA	383	N	LYS	64	46.356	-16.019	65.174	1.00 37.15	В
	ATOM .	384	CA	LYS	64	44.931	-15.788	65.400	1.00 35.14	В
	ATOM									
		385	CB	LYS	64		-14.607	66.342	1.00 36.48	В
	ATOM	386	CG	LYS	64	45.236	-14.826	67.760	1.00 37.70	В
	MOTA	387	CD	LYS	64		-15.510	68.604	1.00 40.04	В
10										
10	ATOM	388	CE	LYS	64	44.488	-15.408	70.087	1.00 40.04	В
	ATOM	389	NZ	LYS	64	43.325	-15.861	70.893	1.00 40.98	В
	ATOM	390		LYS	64					
			C				-15.467	64.041	1.00 33.82	В
	ATOM	391	٥	LYS	64	44.811	-14.590	63.329	1.00 35.17	В
	ATOM	392	N	THR	65	43.253	-16.173	63.669	1.00 31.23	В
15										
13	MOTA	393	CA	THR	65		-15.928	62.377	1.00 30.10	В
	ATOM	394	CB	THR	65	42.784	-17.141	61.438	1.00 32.25	В
	ATOM	395	OG1	THR	65	44.171	-17.498	61.357	1.00 32.66	В
	ATOM	396	CGZ	THR	65	42.2/9	-16.799	60.028	1.00 33.40	В
	ATOM	397	C	THR	65	41.133	-15.597	62.503	1.00 28.24	В
20	ATOM	398	0	THR	65		-16.116	63.382	1.00 28.59	В
	MOTA	399	N	TYR	66	40.648	-14.720	61.630	1.00 24.28	В
	ATOM ·	400	CA	TYR	66	39.244	-14.335	61.665	1.00 22.45	В
	ATOM	401	CB	TYR	66		-12.976	62.362	1.00 19.03	В
~~	ATOM	402	CG	TYR	66	39.783	-12.804	63.674	1.00 16.05	В
25	MOTA	403	CD1	TYR	66	41.158	-12.594	63.697	1.00 11.74	В
	ATOM	404								
				TYR	66		-12.377	64.894		. В
	MOTA	405	CD2	TYR	66	39.094	-12.802	64.891	1.00 15.60	В
	ATOM	406	CE2	TYR	66	39.753	-12.586	66.097	1.00 13.06	В
20	MOTA	407	CZ	TYR	66		-12.368	66.090	1.00 15.20	В
30	MOTA	408	ОН	TYR	66	41.781	-12.100	67.272	1.00 19.72	В
	MOTA	409	С	TYR	66	38 666	-14.241	60.271	1.00 22.39	В
	ATOM	410	0	TYR	66	39.355	-13.876	59.317	1.00 21.02	В
	ATOM	411	N	THR	67	37.387	-14.580	60.167	1.00 23.76	В
	ATOM	412	CA	THR	67			58.900		
25							-14.523		1.00 25.75	В
35	MOTA	413	CB	THR	67	35.789	-15.754	58.699	1.00 24.72	В.
	ATOM	414	OG1	THR	67	36 607	-16.923	58.702	1.00 28.23	В
	MOTA	415		THR	67		-15.664	57.376	1.00 24.97	В
	MOTA	416.	С	THR	67	35.787	-13.291	58.864	1.00 26.39	В
	MOTA	417	0	THR	67		-13.026	59.811	1.00 26.22	В
40										
40	MOTA	418	N	PHE	68	35.899	-12.538	57.775	1.00 26.28	В
	ATOM	419	CA	PHE	68	35.091	-11.342	57.565	1.00 27.23	В
	MOTA	420	CB	PHE	68		-10.056	57.673		
									1.00 25.89	В
	MOTA	421	CG	PHE	68	36.634	-9.893	58.997	1.00 27.52	В
	MOTA	422	CD1	PHE	68	37.873	-10.485	59.230	1.00 26.70	В
45										
73	MOTA	423	CD2		68	36.037	-9.161	60.023	1.00 26.12	В
	ATOM	424	CE1	PHE	- 68	38.501	-10.350	60.464	1.00 25.62	В
	ATOM	425	CE2	PHE	68	36.662	-9.025	61.258	1.00 25.03	В
	ATOM	426	CZ	PHE	68	37.894	-9.619	61.478	1.00 25.92	В
	ATOM	427	C	PHE	68	34.492	-11.434	56.171	1.00 27.19	В
50	MOTA	428	0	PHE	68		-12.206	55.328	1.00 27:43	В
-										
	MOTA	429	N	ASP	69	33.4/0	-10.631	55.926	1.00 26.71	B
	MOTA	430	CA	ASP	69	32.805	-10.629	54.636	1.00 27.55	В
	ATOM .	431	CB	ASP	69	31.660	-9.635	54.684	1.00 27.61	В
65	MOTA	432	CG	ASP	69		-10.019	55.735	1.00 28.58	В
55	MOTA	433	OD1	ASP	69	30.578	-9.403	56.831	1.00 27.66	В
	MOTA	434	OD2		69		-10.972	55.461	1.00 28.48	В
	MOTA	435	С	ASP	69	33.738	-10.366	53.458	1.00 27.41	В
	ATOM	436	0	ASP	69	33.455	-10.771	52.334	1.00 27.23	В
	ATOM									
60		437	N	MET	70	34.861	-9.710	53.732	1.00 28.30	В
60	ATOM	438	CA	MET	70	35.865	-9.396	52.717	1.00 28.88	В
	ATOM	439		MET	70	35.424	-8.213	51.821	1.00 30.69	В
	MOTA	440		MET	70	34.283	-8.469	50.867	1.00 31.73	В
	ATOM	441	SD	MET	70	33.894	-6.957	49.923	1.00 36.68	В
	MOTA	442			70					
65				MET		32.083	-7.049	49.877	1.00 34.73	• В
65	MOTA	443	C	MET	70	37.141	-8.983	53.433	1.00 28.83	В
	MOTA	444	0	MET	70	37.098	-8.480	54.553	1.00 29.82	В
	MOTA	445	N	VAL	71	38.274	-9.188	52.780	1.00 27.33	В
	MOTA	446	CA	VAL	71	39.553	-8.812	53.349	1.00 26.23	В
	ATOM	447	CB	VAL	71		-10.021	54.003	1.00 27.99	
70										В
10	MOTA	448	CG1		71		-10.381	55.319	1.00 28.32	В
	ATOM	449	CG2	VAL	71	40.264	-11.219	53.076	1.00 28.60	В
	ATOM	450	c	VAL	71		-8.233	52.231		
						40.398			1.00 25.01	В
	MOTA	451	0	VAL	71	40.363	-8.713	51.100	1.00 24.55	В

	ATOM	452	N	PHE	72	41.146	-7.191	52.571	1.00 24.93	В
	MOTA	453	ÇA	PHE	72	42.005	-6.475	51.645	1.00 24.43	В
	ATOM	454	CB	PHE	72	41.444	-5.076	51.392	1.00 23.95	В
_	MOTA	455	CG	PHE	72	40.024	-5.059	50.903	1.00 23.17	В
5	ATOM	456	CD1	PHE	72	39.722	-5.376	49.583	1.00 22.75	В
	ATOM	457	CD2	PHE	72	38.991	-4.680	51.754	1.00 23.31	В
	ATOM	458		PHE	72	38.414	-5.310	49.113	1.00 23.87	В
	MOTA	459	CEZ	PHE	72	37.679	-4.612	51.294	1.00 23.71	В
	MOTA	460	CZ	PHE	72	37.389	-4.927	49.970	1.00 24.15	В
10	ATOM	461	С	PHE	72	43.381	-6.321	52.266	1.00 25.11	В
- •			ō		72	43.522				
	MOTA	462		PHE			-5.683	53.312	1.00 26.80	В
	ATOM	463	N	GLY	73	44.394	-6.885	51.621	1.00 24.77	В
	MOTA	464	CA	GLY	73	45.741	-6.774	52.142	1.00 23.03	В
	ATOM	465	С	GLY	73	46.352	-5.450	51.743	1.00 26.33	В
15	MOTA	466	ō	GLY	73	45.698	-4.594	51.141	1.00 26.76	В
10										
	MOTA	467	N	ALA	74	47.626	-5.284	52.062	1.00 27.88	В
	ATOM	468	CA	ALA	74	48.335	-4.054	51.752	1.00 28.98	В
	MOTA	469	CB	ALA	74	49.690	-4.074	52.427	1.00 29.52	В
	ATOM	470	C	ALA	74	48.505	-3.802	50.260	1.00 29.91	В
20	ATOM	471		ALA	74					
20			0			49.037	-2.773	49.865	1.00 31.84	В
	MOTA	472	N	SER	_. 75	48.051	-4.726	49.426	1.00 31.43	В
	ATOM	473	CA	SER	75	48.209	-4.558	47.982	1.00 34.31	В
	MOTA	474	СВ	SER	75	48.382	-5.914	47.318	1.00 32.52	В
	ATOM	475	OG	SER	75	49.088	-6.785	48.183	1.00 36.15	·B
25										
23	MOTA	476	Ç	SER	75	46.994	-3.858	47.395	1.00 34.29	В
	ATOM	477	0	SER	75	47.066	-3.236	46.327	1.00 34.53	В
	ATOM	478	N	THR	76	45.882	-3.963	48.111	1.00 32.69	В
	ATOM	479	CA	THR	76	44.635	-3.364	47.675	1.00 32.77	В
	ATOM	480		THR	76	43.530	-3.549	48.744	1.00 32.84	· B
30										
J U	ATOM	481		THR	76	43.612	-4.863	49.305	1.00 31.95	В
	MOTA	482	CG2	THR	76	42.158	-3.380	48.120	1.00 33.21	В
	ATOM	483	С	THR	76	44.803	-1.870	47.403	1.00 31.46	В
•	ATOM	484	0	THR	76	45.305	-1.134	48.251	1.00 32.33	В
	MOTA	485	N	LYS	77					
35 [°]						44.394	-1.430	46.218	1.00 29.15	В
22	MOTA	486	CA	LYS	77	44.469	-0.015	45.875	1.00 27.33	В
•	MOTA	487	CB	LYS	77	44.906	0.155	44.423	1.00 29.39	В
	ATOM .	488	CG	LYS	77	46.342	-0.341	44.187	1.00 32.84	В
	ATOM	489	CD	LYS		46.949	0.180	42.884	1.00 36.59	В
40	MOTA	490	CE	LYS	77	46.241	-0.349	41.627	1.00 38.03	В
40	MOTA	491	NZ	LYS	77	44.818	0.106	41.501	1.00 38.31	В
	ATOM	492	С	LYS	• 77	43.096	0.625	46.134	1.00 25.52	В
	MOTA	493	0	LYS	77	42.127	-0.088	46.371	1.00 23.25	В
	ATOM	494	N	GLN	78	43.018	1.956	46.115		B
									1.00 24.22	
45	MOTA	495	CA	GLN	78	41.759	2.652	46.398	1.00 22.43	В
45	MOTA	496	CB	GLN	78	41.935	4.177	46.226	1.00 22.53	В
	MOTA	497	CG	GLN	78	43.014	4.799	47.088	1.00 21.23	В
	ATOM	498	CD	GLN	78	42.603	4.953	48.539	1.00 20.15	В
	ATOM	499		GLN	78	42.235	3.988	49.192	1.00 18.03	В
50	MOTA	500	NE2	GLN	78	42.661	6.178	49.045	1.00 21.65	В
50	MOTA	501	C	GLN	78	40.624	2.177	45.504	1.00 22.10	В
	MOTA	502	0	GLN	· 78	39.533	1.839	45.986	1.00 20.46	В
	MOTA	503	N	ILE	79 .	40.898	2.153	44.203	1.00 21.56	В
	MOTA	504	CA	ILE	79	39.929	1.746	43.194	1.00 23.67	В
55	ATOM	505	CB	ILE	79	40.590	1.749	41.774	1.00 23.18	В
22	MOTA	506		ILE	79	41.716	0.732	41.715	1.00 24.28	В
	MOTA	507	CG1	ILE	79	39.574	1.416	40.705	1.00 21.98	В
	MOTA	508	CD1	ILE	79	38.563	2.492	40.470	1.00 23.15	В
		509			-	39.303				_
	MOTA		C	ILE	79 70		0.366	43.475	1.00 25.91	В
C O	ATOM	510	0	ILE	79	38.142	0.120	43.122	1.00 26.57	В
60	MOTA	511	N	ASP	80	40.061	-0.527	44.107	1.00 24.45	В
	MOTA	512	CA	ASP	80	39.547	-1.857	44.416	1.00 25.05	В
	ATOM	513	СВ	ASP	80	40.694	-2.832	44.721	1.00 25.59	В
	ATOM	514	CG	ASP						
					80	41.691	-2.928	43.588	1.00 26.46	В
CE	ATOM	515	OD1		80	41.248	-2.925	42.414	1.00 26.20	В
65	MOTA	516	OD2	ASP	80	42.912	-3.016	43.877	1.00 27.35	В
	MOTA	517	С	ASP	80	38.612	-1.809	45.611	1.00 24.84	В
	MOTA	518	ŏ	ASP	80	37.638	-2.553	45.686		
									1.00 23.83	В
	MOTA	519	N	VAL	81	38.924	-0.934	46.556	1.00 25.12	В
70	MOTA	520	CA	VAL	81	38.102	-0.794	47.742	1.00 25.00	В
70	MOTA	521	CB	VAL	81	38.749	0.174	48.750	1.00 22.43	В
	MOTA	522	CG1		81	37.698	0.713	49.716	1.00 21.58	В
	ATOM	523	CG2		81	39.855	-0.555	49.509	1.00 20.63	В
	MOTA	524	С	VAL	81 ·	36.753	-0.250	47.320	1.00 27.16	В

	MOTA	525	0	VAL	81	35.707	-0.746	47.747	1.00 27.22	В
	MOTA	526	N	TYR	82	36.792	0.769	46.464	1.00 27.98	В
	MOTA	527	CA	TYR	82	35.580	1.406	45.987	1.00 28.04	В
5	MOTA	528	CB	TYR	82	35.922	2.661	45.125	1.00 27.34	В
,	MOTA	529	CG	TYR	82	34.681	3.366	44.637	1.00 26.71	В
	MOTA MOTA	530 531		TYR TYR	82 82	34.262 33.054	3.252 3.808	43.315 42.893	1.00 26.63	B B
	ATOM	532	CD2		82	33.866	4.063	45.529	1.00 27.27	В
	ATOM	533	CE2	TYR	82	32.660		45.128	1.00 28.67	В
10	ATOM	534	cz	TYR	82	32.257	4.488	43.809	1.00 30.95	В
	ATOM	535	ОН	TYR	82	31.047	5.021	43.418	1.00 34.58	· B
	MOTA	536	С	TYR	82	34.705	0.454	45.183	1.00 29.38	В
	ATOM	537	0	TYR	82	33.498	0.322	45.448	1.00 28.44	В
1	MOTA	538	N	ARG	83	35.312	-0.212	44.206	1.00 30.12	В
15	MOTA	539	CA	ARG	83	34.569	-1.136	43.365	1.00 32.33	В
	MOTA	540	CB	ARG	83	35.475	-1.667	42.238	1.00 32.84	В
	MOTA	541	· CG	ARG	83	35.814	-0.610	41.177	1.00 36.78	В
	ATOM ATOM	542 543	CD	ARG	83 83	36.995	-1.024	40.298	1.00 39.59	В
20	ATOM	544	NE C2	ARG ARG	83	36.692 36.158	-2.180 -2.110	39.459 38.242	1.00 45.16	B B
20	MOTA	545		ARG	83	35.870	-0.930	37.706	1.00 47.42	В
	MOTA	546		ARG	83	35.897	-3.226	37.567	1.00 47.17	В
	MOTA	547	C	ARG	83	33.930	-2.291	44.142	1.00 32.86	В
~ ~	MOTA	-548	0	ARG	83	32.786	-2.658	43.866	1.00 34.02	В
25	MOTA	549	N	SER	84	34.648	-2.834	45.125	1.00 32.13	В
	MOTA	550	CA	SER	84	34.159	-3.959	45.933	1.00 30.95	. В
	MOTA	551	-	SER	84	35.347	-4.712	46.558	1.00 32.34	В
	MOTA	552	OG	SER	84	36.301	-5.060	45.568	1.00 37.12	В
30	ATOM ATOM	553	C	SER	84	33.186 32.151	-3.593	47.046	1.00 29.09	В
50	ATOM	554 555	O N	SER VAL	84. 85	33.522	-4.241 -2.570	47.225 47.815	1.00 29.03	B B
	MOTA	556	CA	VAL	85	32.652	-2.176	48.911	1.00 27.74	B
	ATOM	557	СВ	VAL	85	33.481	-1.800	50.165	1.00 25.48	В
	MOTA	558		VAL	85	32.566	-1.623	51.354	1.00 24.98	В
35	MOTA	559	CG2	VAL	85	34.514	-2.865	50.448	1.00 26.13	В.
	MOTA	560	С	VAL	85	31.684	-1.024	48.613	1.00 25.90	В
	MOTA	561	0	VAL	85	30.480	-1.167	48.779	1.00 24.94	В
	MOTA	562	N	VAL	86	32.205	0.106	48.152	1.00 26.94	В
40	MOTA	563	CA	VAL	86	31.368	1.281	47.916	1.00 27.62	В
40	ATOM	564	CB	VAL	86	32.227	2.551	47.793	1.00 25.49	В
	MOTA MOTA	565 566		VAL	86 86	31.384	3.763	48.096	1.00 25.95	В
	MOTA	567	C	VAL VAL	86 86	33.418 30.395	2.480 1.267	48.722 46.736	1.00 24.40 1.00 28.91	B B
	ATOM	568	ŏ	VAL	86	29.254	1.709	46.874	1.00 27.52	В
45	ATOM	569	N	CYS	87	30.835	0.773	45.583	1.00 30.20	В
-	ATOM	570	CA	CYS	87	29.978	0.748	44.402	1.00 31.96	В
	MOTA	571	CB	CYS	87	30.692	0.026	43.257	1.00 35.17	B
	ATOM	572	SG	CYS	87	30.072	0.418	41.599	1.00 41.71	В
50	MOTA	573	Ç	CYS	87	28.593	0.126	44.653	1.00 32.37	В
50	MOTA	574	0	CYS	87	27.571	0.682	44.234	1.00 31.48	В
	MOTA	575	N	PRO	88	28.538	-1.028	45.347	1.00 31.98	В
	ATOM ATOM	576 · 577	CD CA	PRO PRO	88 88	29.675	-1.840 -1.712	45.803	1.00 32.51	В
	MOTA	578	CB	PRO	88	27.272 27.720	-3.024	45.648 46.269	1.00 30.72 1.00 31.27	B B
55	MOTA	579	CG	PRO	88	29.104	-3.024	45.739	1.00 32.03	В
	MOTA	580	c	PRO	. 88	26.407	-0.907	46.617	1.00 30.37	В
	MOTA	581	ō	PRO	88	25.179	-0.928	46.528	1.00 29.46	B
	ATOM	582	N	ILE	89	27.060	-0.214	47.549	1.00 28.89	В
	ATOM	583	CA	ILE	89	26.372	0.607	48.539	1.00 26.92	В
60	ATOM	584	CB	ILE	89	27.325	1.032	49.677	1.00 27.36	В
	MOTA	585		ILE	89	26.562	1.827	50.728	1.00 29.65	В
	MOTA	586		ILE	89	27.949	-0.202	50.327	1.00 28.47	В
	ATOM	587	CD1		89	28.880	0.116	51.493	1.00 28.07	В
65	ATOM	588	C	ILE	89	25.815	1.866	47.883	1.00 26.45	В
UJ	ATOM	589	0	ILE	89	24.733	2.329	48.236	1.00 25.57	В
	ATOM	590	N	LEU	90	26.551	2.416	46.922	1.00 26.88	В
	ATOM ATOM	591 592	CA CB	LEU	90 90	26.097 27.185	3.618 4.167	46.242 45.305	1.00 27.21 1.00 26.30	B
	ATOM	592 593	CG	LEU	90	26.768	5.457	45.305	1.00 26.30	B
70	ATOM	594	CD1		90	26.300	6.546	45.499	1.00 27.39	. В
. •	ATOM	595	CD2		90	27.936	5.952	43.707	1.00 30.13	В
	ATOM	596	c	LEU	90	24.828	3.334	45.451	1.00 28.12	В
	MOTA	597	ō	LEU	90	23.914	4.156	45.423	1.00 27.80	В

	ATOM	598	N	ASP	.91	24.778	2.168	44.811	1.00 29.04	В
	MOTA	599	CA	ASP	91	23.615	1.782	44.029	1.00 29.68	В
	ATOM	600	CB	ASP	91	23.888	0.479	43.238	1.00 30.25	В
_	MOTA	601	CG	ASP	91	24.715	0.717	41.975	1.00 33.21	В
5	MOTA	602	OD1	ASP	91	24.655	1.836	41.417	1.00 33.99	• В
	MOTA	603		ASP	91	25.409	-0.225	41.522	1.00 34.57	В
	MOTA	604	С	ASP	91	22.412	1.604	44.950	1.00 29.79	В
	MOTA	605	0	ASP	91	21.265	1.785	44.542	1.00 29.34	B
10	MOTA	606	N	GLU	92	22.684	.1.254	46.199	1.00 30.26	В
10	MOTA	607	CA	GLU	92	21.632	1.077	47.191	1.00 33.20	В
	MOTA	608	·CB	GLU	92	22.240	0.434	48.455	1.00 37.58	В
	MOTA	609	CG	GLU	92	21.243	-0.021	49.519	1.00 45.34	В
	MOTA	610	CD	GLU	92	20.622	-1.378	49.215	1.00 49.33	В
15	ATOM	611		GLU	92	19.996	-1.963	50.134	1.00 51.49	В
13	MOTA	612		GLU	92	20.760	-1.851	48.061	1.00 50.48	В
	MOTA	613	C	GLU	92 92	21.036	2.471	47.516	1.00 32.34	В
	MOTA MOTA	614 615	O N	GLU VAL	92	19.816 21.921	2.659 3.438	47.548 47.757	1.00 31.40 1.00 29.83	B B
	MOTA	616	CA	VAL	93	21.521	4.813	48.060	1.00 27.09	В
20	MOTA	617	CB	VAL	93	22.794	5.732	48.216	1.00 27.00	В
	MOTA	618	CG1		93	22.362	7.185	48.503	1.00 23.70	В
	ATOM	619	CG2		93	23.720	5.189	49.320	1.00 24.02	В
	ATOM	620	c	VAL	93	20.661	5.384	46.936	1.00 25.06	B.
	ATOM	621	ŏ	VAL	93	19.631	6.005	47.184	1.00 23.16	·B
25	MOTA	622	N	ILE	94	21.090	5.173	45.700	1.00 23.81	В
	MOTA	623	CA	ILE	94	20.357	5.679	44.554	1.00 26.20	В
	ATOM	624	CB	ILE	94	21.196	5.496	43.268	1.00 24.09	В
	MOTA	625	CG2	ILE	94 .	20.398	5.871	42.040	1.00 22.58	В
20	MOTA	626	CG1		94	22.436	6.394	43.367	1.00 23.30	В
30	MOTA	627	CD1		94	23.378	6.288	42.211	1.00 25.19	В
	MOTA	628	С	ILE	94	18.964	5.057	44.417	1.00 28.52	В
	MOTA	629	0	ILE	94	18.101	5.606	43.742	1.00 30.41	В
	MOTA	630	N	MET	95	18.729	3.925	45.073	1.00 31.00	В
35	ATOM	631	ÇA	MET	95	17.408	3.305	45.032	1.00 32.10	В
رد	MOTA	632	CB	MET	95	17.501	1.789	45.171	1.00 35.87	В
•	ATOM	633	CG	MET MET	95 95	17.836	1.059	43.885	1.00 39.09	В
	ATOM	634	SD	MET	95 95	17.725	-0.743	44.078	1.00 46.44	В
	MOTA MOTA	635 636	C	MET	95	19.451 16.514	-1.155 3.857	44.567 46.140	1.00 42.73 1.00 31.79	B B
40	ATOM	637	Ö	MET	95	15.340	3.518	46.204	1.00 32.44	В
	MOTA	638	N	GLY	96	17.069	4.697	47.016	1.00 31.15	В
	MOTA	639	CA	GLY	96	16.274	5.290	48 083	1.00 30.86	В
	ATOM	640	c	GLY	96	16.506	4.778	49.497	1.00 31.33	В
	ATOM	641	0	GLY	96	15.695	5.005	50.398	1.00 31.96	В
45	MOTA	642	N	TYR	97	17.617	4.085	49.700	1.00 31.69	В
	ATOM	643	CA	TYR	97	17.951	3.539	51.009	1.00 31.47	В
	MOTA	644	CB	TYR	97	18.620	2.119	50.859	1.00 35.21	В
	MOTA	645	CG	TYR	. 97	17.707	0.979	50.448	1.00 38.09	В
50	MOTA	646		TYR	97	16.856	0.369	51.374	1.00 38.78	В
50	MOTA	647	CE1		97	16.060	-0.716	51.017	1.00 39.92	В
	MOTA	648	CD2		97	17.733	0.476	49.146	1.00 38.17	В
	MOTA	649	CE2		97	16.938	-0.606	48.777	1.00 40.59	В
	ATOM	650	CZ	TYR	97 07	16.105	-1.197	49.717	1.00 42.01	В
55	MOTA MOTA	651 652	OH	TYR TYR	97 97	15.314 18.944	-2.262	49.350	1.00 44.26 1.00 29.27	В
55	MOTA	653	õ	TYR	97	19.557	4.465 5.309	51.699		B B
	ATOM	654	N	ASN	98	19.089		51.055 53.008	1.00 29.87	
	ATOM	655	CA	ASN	98	20.061	4.308 5.081	53.768	1.00 26.93 1.00 27.11	B B.
	ATOM	656	CB	ASN	98	19.500	5.509	55.156	1.00 27.11	В
60	ATOM	657	CG	ASN	98	18.435	6.579	55.048	1.00 27.12	В
	MOTA	658	OD1		98	18.553	7.506	54.245	1.00 30.11	В
	ATOM	659		ASN	98	17.394	6.465	55.860	1.00 26.60	В
	ATOM	660	C	ASN	98	21.243	4.141	53.975	1.00 26.22	В
	ATOM	661	ō	ASN	98	21.055	2.971	54.292	1.00 25.58	В
65	ATOM	662	N	CYS	99	22.457	4.634	53.775	1.00 25.47	В
	MOTA	663	CA	CYS	99	23.629	3.791	53.977	1.00 25.10	В
	MOTA	664	CB	CYS	99	24.206	3.357	52.654	1.00 26.81	В
	MOTA	665	SG	CYS	99	23.084	2.317	51.714	1.00 26.81	В
70	MOTA	666	С	CYS	99	24.697	4.486	54.798	1.00 23.75	В
70	MOTA	667	0	CYS	99	24.804	5.712	54.804	1.00 25.67	В
	MOTA	668	N	THR	100	25.482	3.683	55.496	1.00 20.94	В
	MOTA	669	CA	THR	100	26.549	4.181	56.341	1.00 19.27	В
	MOTA	670	CB	THR	100	26.076	4.266	57.795	1.00 17.86	В

	MOTA	671	0G1	THR	100	24.992	5.192	57.875	1.00 16.90	В
	MOTA	672	CG2	THR	100	27.202	4.714	58.708	1.00 17.10	В
	ATOM	673	C	THR	100	27.760	3.247	56.269	1.00 19.78	В
	MOTA	674	ŏ	THR	100	27.615	2.013	56.297	1.00 19.41	В
5										
,	MOTA	675	N	ILE	101	28.945	3.846	56.170	1.00 17.12	В
	MOTA	676	CA	ILE	101	30.194	3.096	56.112	1.00 13.84	• В
	ATOM	677	CB	ILE	101	30.923	3.273	54.770	1.00 11.63	В
	MOTA	678	CG2	ILE	101	32.193	2.459	54.763	1.00 11.54	В
	ATOM	679	CG1	ILE	101	30.029	2.847	53.614	1.00 11.12	В
10	MOTA	680		ILE	101	30.610	3.205	52.240	1.00 8.60	В
	MOTA	681	Č	ILE	101	31.088	3.655	57.189	1.00 14.61	. в
	MOTA	682	0	ILE	101	31.434	4.828	57.158	1.00 16.06	В
	MOTA	683	N	PHE	102	31.454	2.814	58.149	1.00 16.69	В
	MOTA	684	CA	PHE	102	32.336	3.214	59.246	1.00 15.45	В
15	MOTA	685	CB	PHE	102	31.957	2.509	60.517	1.00 15.38	В
	ATOM	686	CG	PHE	102	30.704	3.002	61.158	1.00 17.02	В
	ATOM	687	· CD1		102	30.746	4.068	62.060	1.00 14.70	В
	MOTA	688		PHE	102	29.489	2.341	60.937	1.00 15.06	В
	ATOM	689		PHE	102	29.601	4.468	62.744		В
20									1.00 15.17	
20	MOTA	690		PHE	102	28.336	2.732	61.614	1.00 16.46	В
	MOTA	691	CZ	PHE	102	28.389	3.797	62.523	1.00 16.06	В
	ATOM	692	C	PHE	102	33.770	2.789	58.956	1.00 13.66	В
	MOTA	693	0	PHE	102	34.004	1.767	58.335	1.00 14.29	В
	ATOM	694	N	ALA	103	34.723	3.571	59.431	1.00 14.00	В
25	MOTA	695	CA	ALA	103	36.135	3.230	59.309	1.00 13.68	В
	ATOM	696	CB	ALA	103	36.894	4.316	58.595	1.00 12.73	. В
	ATOM	697		ALA	103	36.579	3.142	60.771	1.00 14.68	
			Ċ							В
	MOTA	698	0	ALA	103	36.560	4.144	61.491	1.00 12.81	
20	MOTA	699	N	TYR	104	36.943	1.939	61.211	1.00 14.23	В
30	ATOM	700	CA	TYR	104	37.369	1.722	62.588	1.00 13.28	В
	ATOM	701	CB	TYR	104	36.415	0.741	63.271	1.00 13.08	В
	MOTA	702	CG	TYR	104	36.704	0.496	64.740	1.00 9.23	В
	ATOM	703		TYR	104 .	37.774	-0.304	65.139	1.00 10.77	В
	ATOM	704	CE1		104	38.050	-0.519	66.497	1.00 8.87	В
35										
25	MOTA	705		TYR	104	35.916	1.072	65.728	1.00 7.28	В
	MOTA	706	CE2	TYR	104	36.180	0.861	67.085	1.00 6.26	B
	MOTA	707	CZ	TYR	104	37.245	0.063	67.459	1.00 6.63	В
	MOTA	708	OH	TYR	104	37.492	-0.189	68.791	1.00 6.91	В
	ATOM	709	С	TYR	104	38.791	1.191	62.660	1.00 14.55	В
40	MOTA	710	0	TYR	104	39.192	0.344	61.866	1.00 17.36	B
	ATOM	711	N	GLY	105	39.553	1.688	63.622	1.00 15.00	В
	ATOM	712	CA	GLY	105	40.920	1.239	63.760	1.00 16.15	В
	MOTA	713	C	GLY	105	41.818	2.222	64.480	1.00 18.48	В
15	MOTA	714	0	GLY	105	41.464	3.383	64.733	1.00 19.06	В
45	MOTA	715	N	GLN	106	42.996	1.726	64.818	1.00 18.69	В
	ATOM	716	CA	GLN	106	44.012	2.480	65.524	1.00 20.40	В
	MOTA	717	CB	GLN	106	45.109	1.510	65.958	1.00 20.92	В
	ATOM	718	CG	GLN	106	46.494	2.093	65.959	1.00 25.11	В
	ATOM	719	CD	GLN	106	47.546	1.104	66.424	1.00 27.12	B
50	ATOM	720		GLN	106	47.724	0.033	65.833	1.00 29.47	В
50	ATOM	721		GLN	106					
						48.254	1.462	67.486	1.00 24.05	В
	ATOM	722	C	GLN	106	44.595	3.602	64.668	1.00 22.74	В
	MOTA	723	0	GLN	106	44.733	3.442	63.447	1.00 22.56	В
سر سر	MOTA	724	N	THR	107	44.924	4.733	65.312	1.00 22.64	В
55	ATOM	725	CA	THR	107	45.526	5.893	64.637	1.00 21.79	В
	ATOM	726	CB	THR	107	46.070	6.943	65.659	1.00 22.17	В
	ATOM	727		THR	107	45.014	7.404	66.510	1.00 22.36	В
	ATOM	728	CG2		107	46.675	8.142	64.927	1.00 19.97	В
		729								
60	ATOM		C	THR	107	46.720	5.430	63.788	1.00 21.90	. В
00	ATOM	730	0	THR	107	47.605	4.752	64.288	1.00 20.99	В
	MOTA	731	N	GLY	108	46.739	5.796	62.510	1.00 22.46	В
	MOTA	732	CA	GLY	108	47.836	5.394	61.652	1.00 21.62	В
	ATOM	733	С	GLY	108	47.664	4.088	60.882	1.00 22.90	В
	ATOM	734	0	GLY	108	48.653	3.547	60.376	1.00 24.07	В
65	MOTA	735	N	THR	109	46.436	3.572	60.786	1.00 22.29	В
	MOTA	736	CA	THR	109	46.197	2.321	60.050	1.00 21.18	
										В
	MOTA	737	CB	THR	109	45.408	1.259	60.884	1.00 21.26	В
	ATOM	738		THR	109	44.159	1.814	61.335	1.00 20.11	В
70	ATOM	739		THR	109	46.250	0.777	62.071	1.00 19.60	В
70	ATOM	740	С	THR	109	45.439	2.523	58.754	1.00 19.58	В
	MOTA	741	0	THR	109	45.126	1.551	58.068	1.00 20.97	В
	ATOM	742	N	GLY	110	45.125	3.776	58.428	1.00 17.22	В
	ATOM	743	CA	GLY	110	44.415	4.048	57.193	1.00 12.69	В
	711 017	, 13	~^				4.040	51.193	1.00 12.09	Ð

	MOTA	744	С	GLY	110	42.943	4.424	57.232	1.00 12.29	В
	ATOM	745	ŏ	GLY	110	42.288	4.365	56.193	1.00 14.37	В
	ATOM	746	N	LYS	111	42.398	4.795	58,386	1.00 11.41	В
_	ATOM	747	CA	LYS	111	40.983	5.198	58.432	1.00 12.47	В
5	MOTA	748	СB	LYS	111	40.540	5.653	59.898	1.00 13.24	В
	MOTA	749	CG	LYS	111	40.379	4.538	60.934	1.00 10.82	В
	MOTA	750	CD	LYS	111	39.805	5.061	62.229	1.00 6.09	В
•	MOTA	751	CE	LYS	111	40.691	6.142	62.813	1.00 10.33	В
10	MOTA	752	NZ	LYS	111	42.130	5.748	63.038	1.00 9.60	В
10	MOTA	753	C	LYS	111	40.742	6.363	57.465	1.00 13.44	В
	MOTA	754	.0	LYS	111	39.870	6.295	56.587	1.00 14.48	В
	MOTA MOTA	755 756	N CA	THR THR	112 112	41.538	7.423 8.613	57.614	1.00 14.82	В
•	MOTA	757	CB	THR	112	41.403	9.793	56.773 57.417	1.00 15.93 1.00 15.93	В
15	ATOM	758		THR	112	41.538	10.066	58.694	1.00 13.93	B B
	ATOM	759		THR	112	42.055	11.040	56.522	1.00 13.41	В
•	ATOM	760	C	THR	112	41.870	8.426	55.323	1.00 17.21	В
	MOTA	761	Õ	THR	112	41.318	9.021	54.385	1.00 16.82	В
	MOTA	762	N	PHE	113	42.887	7.595	55.142	1.00 17.40	В
20	MOTA	763	CA	PHE	113	43.398	7.313	53.811	1.00 16.82	В
	MOTA	764	CB	PHE	113	44.654	6.389	53.889	1.00 16.02	В
	MOTA	765	CG	PHE	113	45.233	6.054	52.540	1.00 17.10	В.
	MOTA	766		PHE	113	46.126	6.918	51.920	1.00 18.15	В
25	MOTA	.767		PHE	113	44.836	4.911	51.868	1.00 18.15	В
23	MOTA	768		PHE	113	46.614	6.654	50.652	1.00 19.37	В
	ATOM ATOM	769 770	CEZ	PHE	113	45.317	4.632	50.588	1.00 20.77	В
	ATOM	771	c	PHE	113 113	46.208	5.508 6.615	49.980	1.00 21.58	В
	ATOM	772	ò	PHE	113	42.125	6.894	52.997 51.816	1.00 15.35	B
30	ATOM	773	N	THR	114	41.590	5.700	53.647	1.00 14.49	В
	MOTA	774	CA	THR	114	40.524	4.942	53.008	1.00 13.72	В
	ATOM	775	CB	THR	114	40.119	3.722	53.868	1.00 14.47	В
	MOTA	776		THR	114	41.228	2.834	53.980	1.00 13.50	В
25	MOTA	777		THR	114	38.944	2.984	53.258	1.00 10.99	В
35	MOTA	778	C	THR	114	39.283	5.773	52.764	1.00 13.62	В
•	MOTA	779	0	THR	114	38.733	5.758	51.674	1.00 14.61	В
	MOTA MOTA	780 781	N CA	MET	115 115	38.842	6.499	53.784	1.00 15.54	В
	ATOM	782	CB	MET	115	37.635 37.121	7.311	53.663 55.043	1.00 16.98 1.00 17.73	B B
40	MOTA	783	CG	MET	115	36.776	6.525	55.938	1.00 17.73	В
	ATOM	784	SD	MET	115	35.694	5.280	55.139	1.00 24.33	В
	MOTA	785	CE	MET	115	34.110	6.102	55.162	1.00 17.96	В
	MOTA	786	C	MET	115	37.772	8.556	52.809	1.00 16.94	В
45	MOTA	787	0	MET	115	36.824	8.956	52.140	1.00 17.35	В
43	ATOM	788	N	GLU	116	38.947	9.168	52.816	1.00 16.96	В
	MOTA MOTA	789 790	CA	GLU	116	39.139	10.391	52.040	1.00 17.40	В
	ATOM	791	CB CG	GLU	116 116	39.564 38.457	11.563 12.038	52.988	1.00 17.75	В
	ATOM	792	CD.	GLU	116	38.980	12.893	53.929 55.070	1.00 20.71	B B
50	ATOM	793		GLU	116	40.113	13.404	54.961	1.00 26.78	В
	MOTA	794		GLU	116	38.260	13.064	56.074	1.00 22.44	В
	ATOM	795	С	GLU	116	40.178	10.211	50.953	1.00 16.14	В
	MOTA	796	0	GLU	116	39.925°	10.474	49.783	1.00 12.66	В
55	MOTA	797	N	GLY	117	41.357	9.768	51.360	1.00 16.93	В
23	ATOM	798	CA	GLY	117	42.425	9.585	50.406	1.00 21.10	В
	MOTA MOTA	799 800	C	GLY	117	43.424	10.723	50.439	1.00 22.08	В
	ATOM	801	N	GLY GLU	117 118	43.321 44.390	11.640 10.661	51.248 49.536	1.00 21.52	В
	ATOM	802	CA	GLU	118	45.436	11.664	49.336	1.00 24.00 1.00 26.12	В.
60	MOTA	803	СВ	GLU	118	46:712	11.116	50.134	1.00 27.39	B B
	ATOM	804	CG	GLU	118	46.574	11.023	51.647	1.00 32.78	В
	ATOM	805	CD	GLU	118	47.603	10.111	52.316	1.00 37.03	В
	MOTA	806	OE1		118	48.799	10.149	51.938	1.00 36.38	В
45	MOTA	807	OE2		118	47.208	9.369	53.246	1.00 39.57	В
65	MOTA	808	C	GLU	118	45.702	12.026	48.000	1.00 26.11	В
	MOTA	809	0	GLU	118	45.079	11.481	47.088	1.00 24.83	В
	ATOM ATOM	810 811	N	ARG	119	46.613	12.961	47.780	1.00 25.93	В
	ATOM	812	CA CB	ARG ARG	119 119	46.922 47.076	13.355 14.913	46.423 46.313	1.00 26.49	В
70	ATOM	813	CG	ARG	119	45.824	15.737	46.513	1.00 24.19 1.00 18.83	B B
-	ATOM	814	CD	ARG	119	44.579	15.206	45.965	1.00 15.06	. 18
	ATOM	815	NE	ARG	119	44.755	14.940	44.542	1.00 15.80	В
	MOTA	816	CZ	ARG	119	44.761	15.869	43.591	1.00 18.90	В

	АТОМ	817	NT//1	ARG	119	44 601	17 142	42 010	1 00 20 61	-
	ATOM	818		ARG	119	44.601 44.910	17.142 15.528	43.910 42.314	1.00 20.61 1.00 17.87	B B
	ATOM	819	Ċ	ARG	119	48.207	12.682	45.967	1.00 29.08	B
_	ATOM	820	ō	ARG	119	49.178	12.572	46.735	1.00 27.84	В
5	ATOM	821	N	SER	120	48.205	12.192	44.731	1.00 30.37	В
	MOTA	822	CA	SER	120	49.417	11.597	44.203	1.00 32.15	В
	MOTA	823	CB	SER	120	49.190	11.014	42.825	1.00 33.55	В
	MOTA	824	OG	SER	120	48.380	9.854	42.897	1.00 34.65	В
10	ATOM	825	C	SER	120		12.839	44.123	1.00 31.39	В
10	ATOM ATOM	826 827	O N	SER PRO	120 121	49.849 51.522	13.883 12.745	43.651 44.599	1.00 31.19	В
	MOTA	828	CD	PRO	121	52.207	11.494	44.965	1.00 30.67	В
	MOTA	829	CA	PRO	121	52.455	13.870	44.595	1.00 31.71	В
	ATOM	830	СВ	PRO	121	53.674	13.288	45.270	1.00 31.87	В
15	MOTA	831	CG	PRO	121 .	53.658	11.869	44.783	1.00 32.88	В
	ATOM	832	С	PRO	121 .		14.511	43.240	1.00 32.30	В
	MOTA		. 0	PRO	121	52.557	13.925	42.176	1.00 32.32	B
	MOTA	834	N	ASN	122	53.319	15.733	43.319	1.00 30.43	В
20	MOTA MOTA	835 836	CA	ASN	122	53.753	16.529	42.175	1.00 30.58	В
20	ATOM	837	CB CG	ASN ASN	122 122	54.974 56.101	15.864 16.850	41.515 41.250	1.00 30.83 1.00 29.55	B B
	ATOM .	838	OD1		122	56.512	17.589	42.139	1.00 30.20	В
	ATOM	839	ND2		122	56.614	16.849	40.032	1.00 29.25	В
~-	ATOM	840	С	ASN	122	52.708	16.838	41.107	1.00 30.96	В
25	ATOM	841	0	ASN	122	53.022	16.840	39.916	1.00 28.89	· B
	MOTA	842	N	GLU	123	51.479	17.121	41.540	1.00 31.29	. В
	ATOM	843		GLU	123	50.380	17.435	40.630	1.00 31.61	В
	ATOM ATOM	844 845	CB	GLU	123	50.437	18.873	40.222	1.00 29.75	В
30	ATOM	846	CG CD	GLU GLU	123 123	50.311 50.030	19.825 21.243	41.382 40.942	1.00 31.53	B B
•	MOTA	847	OE1		123	50.896	21.842	40.255	1.00 32.81	В
	ATOM	848	OE2		123	48.937	21.753	41.288	1.00 35.74	В
	ATOM	849	С	GLU	123	50.396	16.558	39.393	1.00 32.07	В
25	ATOM	850	0	GLU	123	50.246	17.038	38.272	1.00 32.39	В
35	MOTA	851	N	GLU	124	50.576	15.261	39.620	1.00 33.92	В.
	MOTA	852	CA	GLU	124	50.628	14.269	38.558	1.00 33.69	В
	ATOM ATOM	853 854	CB CG	GLU	124	51.235	12.998	39.111	1.00 35.39	В
	ATOM	855	CD	GLU	124 124	51.234 51.966	11.798 10.613	38.184 38.801	1.00 39.45 1.00 42.18	B B
40	ATOM	856	OE1		124	51.802	10.390	40.026	1.00 42.18	B
-	ATOM	857		GLU	124	52.698	9.906	38.067	1.00 42.46	В
	ATOM	858	С	GLU	124	49.252	13.994	37.958	1.00 33.48	В
	ATOM	859	0	GLU	124	49.149	13.665	36.778	1.00 33.85	В
45	MOTA	860	N	TYR	125	48.196	14.141	38.758	1.00 32.64	В
43	ATOM ATOM	861 862	CA	TYR TYR	125	46.841	13.895	38.267	1.00 33.52	В
	MOTA	863	CB	TYR	125 125	46.261 47.109	12.523 11.290	38.817 38.613	1.00 33.48 1.00 35.23	B B
	ATOM	864		TYR	125	47.951	10.826	39.624	1.00 35.75	В
	ATOM	865		TYR	125	48.709	9.668	39.461	1.00 36.41	В
50	ATOM	866	CD2	TYR	125	47.046	10.565	37.422	1.00 36.88	В
	ATOM	867		TYR	125	47.803	9.403	37.242	1.00 37.22	В
	MOTA	868	CZ	TYR	125	48.630	8.962	38.268	1.00 38.72	В
	ATOM	869	ОН	TYR	125	49.369	7.811	38.108	1.00 40.27	В
55	ATOM ATOM	870 871	С 0	TYR TYR	125 125	45.851 46.150	14.985 15.834	38.677 39.520	1.00 33.79 1.00 34.63	B B
-	ATOM	872	N	THR	126	44.669	14.949	38.063	1.00 33.04	В
	ATOM	873	CA	THR	126	43.588	15.858	38.420	1.00 31.85	В
	ATOM	874	CB	THR	126	42.562	16.061	37.286	1.00 31.42	В
60	ATOM	875	OG1		126	42.214	14.790	36.723	1.00 29.37	· в
60	ATOM	876	CG2		126	43.114	16.996	36.216	1.00 30.94	В
	ATOM	877	Ç	THR	126	42.911	15.061	39.518	1.00 31.76	В
	ATOM	878	0	THR	126	43.023	13.836	39.552	1.00 31.47	В
	ATOM ATOM	879 880	N CA	TRP TRP	127 127	42.197 41.559	15.738 15.053	40.401 41.507	1.00 31.44	В
65	MOTA	881	CB	TRP	127	40.749	16.048	42.357	1.00 30.17	B B
	ATOM	882	CG	TRP	127	39.474	16.455	41.718	1.00 25.01	В
	ATOM	883	CD2		127	38.207	15.796	41.846	1.00 24.45	В
	MOTA	884	CE2	TRP	127	37.285	16.514	41.059	1.00 24.12	В
70	ATOM	885	CE3		127	37.764	14.662	42.546	1.00 22.04	В
70	ATOM	886	CD1		127	39.278	17.507	40.885	1.00 23.64	В
	ATOM ATOM	887 888	NE1 CZ2		127	37.966	17.553	40.483	1.00 24.14	В
	ATOM	889	CZ2		127 127	35.937 36.427	16.143 14.285	40.952 42.441	1.00 25.81 1.00 24.07	B B
						/				

	ATOM	890	CH2	TRP	127	35.526	15.026	41.647	1.00 26.19	В
	MOTA	891	C	TRP	127	40.664	13.883	41.099	1.00 30.31	В
	MOTA	892	0	TRP	127	40.635	12.859	41.784	1.00 31.25	В
	MOTA	893	N	GLU	128	39.945	14.014	39.991	1.00 30.25	В
5	ATOM	894	ĊA	GLU	128	39.036	12.943	39.575	1.00 29.93	В
•	ATOM	895	CB	GLU	128	38.010	13.477	38.601	1.00 30.66	В
	ATOM		CG	GLU	128	38.597	14.116	37.360	1.00 30.88	В
	ATOM	897	CD	GLU						
					128	37.522	14.757	36.522	1.00 37.02	В
10	ATOM	898		GLU	128	36.740	15.558	37.085	1.00 37.94	В
10	ATOM	899		GLU	128	37.450	14.460	35.309	1.00 39.71	В
	MOTA	900	Ċ	GLU	128	39.692	11.704	38.977	1.00 28.41	В
	ATOM	901	0	GLU	128	39.004	10.755	38.623	1.00 28.40	В
	MOTA	902	N	GLU	129	41.012	11.716	38.853	1.00 27.73	В
	MOTA	903	CA	GLU	129	41.724	10.574	38.303	1.00 26.98	В
15	MOTA	904	CB	GLU	129	42.343	10.919	36.940	1.00 25.80	В
	ATOM	905	CG	GLU	129	41.317	11.144	35.841	1.00 28.03	В
	ATOM	906	CD	GLU	129	41.954	11.422	34.487	1.00 33.17	В
	ATOM	907		GLU	129	41.201	11.654	33.510	1.00 35.80	В
	MOTA	908		GLU	129	43.206	11.411	34.389	1.00 33.00	В
20	ATOM	909	C	GLU	129	42.807	10.110	39.257	1.00 33.31	. B
	ATOM	910	ŏ	GLU	129	43.480	9.117			
	ATOM	911	N	ASP	130			38.997	1.00 28.14	В
						42.966	10.814	40.372	1.00 27.13	В.
	MOTA	912	CA	ASP	130	43.995	10.445	41.336	1.00 28.16	В
25	MOTA	.913	СВ	ASP	130	44.092	11.498	42.458	1.00 29.19	·B
23	MOTA	914	CG	ASP	130	45.484	11.577	43.061	1.00 31.28	В
	MOTA	915		ASP	130	46.026	10.525	43.470	1.00 31.52	В
	MOTA	916		ASP	130	46.039	12.695	43.125	1.00 33.01	В
	MOTA	917	C	ASP	130	43.690	9.068	41.925	1.00 27.22	В
20	MOTA	918	Ó	ASP	130	42.646	8.865	42.551	1.00 27.12	В
30	MOTA	919	N	PRO	131	44.590	8.093	41.704	1.00 26.27	В
	MOTA	920	CD	PRO	131	45.722	8.143	40.760	1.00 25.74	В
	ATOM	921	CA	PRO	131	44.404	6.733	42.217	1.00 25.42	В
	MOTA	922	CB	PRO	131	45.436	5.928	41.431	1.00 25.20	В
. _	MOTA	923	CG	PRO	131	46.516	6.926	41.158	1.00 25.28	В
35	MOTA	. 924	С	PRO	131	44.550	6.586	43.734	1.00 25.10	В
	MOTA	925	0	PRO	131	44.317	5.514	44.284	1.00 25.70	В
	MOTA	926	N	LEU	132	44.939	7.659	44.414	1.00 25.55	В
	MOTA	927	CA	LEU	132		7.615	45.870	1.00 24.12	В
	ATOM	928	CB	LEU	132	46.335	8.393	46.358	1.00 23.33	В
40	ATOM	929	CG	LEU	132	47.750	7.835	45.985	1.00 24.01	В
	ATOM	930		LEU	132	48.853	8.699	46.613	1.00 21.35	
	MOTA	931		LEU	132	47.875				В
	ATOM	932	CDZ	LEU			6.394	46.474	1.00 25.49	В
					132	43.794	8.216	46.497	1.00 23.99	В
45	ATOM	933	0	LEU	132	43.694	8.338	47.728	1.00 24.50	В
43	ATOM	934	N	ALA	133	42.831	8.587	45.650	1.00 21.97	В
	MOTA	935	CA	ALA	133	41.566	9.155	46.129	1.00 23.50	В
	MOTA	936	CB	ALA	133	40.738	9.710	44.958	1.00 19.96	В
	MOTA	937	C	ALA	133	40.760	8.097	46.896	1.00 24.12	В
50	MOTA	938	0	ALA	133	40.766	6.914	46.552	1.00 24.63	В
50	MOTA	939	N	GLY	134	40.060	8.546	47.931	1.00 25.21	В
	MOTA	940	CA	GLY	134	39.289	7.646	48.763	1.00 23.61	В
	ATOM	941	С	GLY	134	37.831	7.541	48.387	1.00 23.90	В
	ATOM	942	0	GLY	134	37.399	8.030	47.344	1.00 25.12	В
~ ~	ATOM	943	N	ILE	135	37.075	6.887	49.261	1.00 22.33	В
55	ATOM	944	CA	ILE	135	35.657	6.662	49.055	1.00 19.60	В
	ATOM	945	CB	ILE	135	35.048	5.962	50.295	1.00 17.94	В
	ATOM	946	CG2	ILE	135	33.513	5.984			В
	ATOM	947	CG1		135	35.604	4.531	50.381	1.00 13.85	В
	ATOM	948	CD1		135	35.402	3.883	51.712	1.00 11.57	B
60	MOTA	949	C	ILE	135	34.886	7.941	48.751	1.00 19.64	В
	ATOM	950	ŏ	ILE	135	34.130	7.995	47.789	1.00 17.27	В
	ATOM	951	N	ILE	136	35.090	8.971	49.566	1.00 19.64	В
	ATOM	952	CA	ILE	136	34.383	10.229	49.377	1.00 19.00	
	ATOM	953	CB	ILE	136	34.758	11.219	50.486		В
65		954							1.00 18.34	В
5.7	MOTA		CG2		136	34.174	12.595	50.188	1.00 19.49	В
	MOTA	955	CG1		136	34.226	10.669	51.838	1.00 18.91	В
	MOTA	956	CD1		136	34.680	11.447	53.086	1.00 18.92	В
	ATOM	957	C	ILE	136	34.552	10.867	47.991	1.00 17.37	В
70	MOTA	958	0	ILE	136	33.614	10.888	47.207	1.00 15.94	В
10	MOTA	959	N	PRO	137	35.742	11.382	47.662	1.00 16.74	В
	MOTA	960	CD	PRO	137	37.083	11.311	48.259	1.00 16.29	В
	MOTA	961	CA	PRO	137	35.785	11.963	46.318	1.00 17.68	В
	MOTA	962	CB	PRO	137	37.263	12.305	46.132	1.00 14.17	В

	ATOM	963	CG	PRO	137	37.966	11.351	47.037	1.00 16.06	В
	MOTA	964	C	PRO	137	35.229	11.025	45.232	1.00 20.66	В
	MOTA	965	0	PRO	137	34.408	11.434	44.406	1.00 22.43	В
5	MOTA MOTA	966 967	N CA	ARG ARG	138 138	35.651 35.154	9.764 8.825	45.232 44.224	1.00 21.33 1.00 21.16	B B
	ATOM	968	CB	ARG	138	35.768	7.428	44.436	1.00 19.87	В
	ATOM	969	CG	ARG	138	37.251	7.370	44.138	1.00 18.07	B
	ATOM	970	CD	ARG	138	37.812	5.989	44.402	1.00 17.00	В
	ATOM	971	NE	ARG	138	39.264	6.019	44.408	1.00 14.48	В
10	MOTA	972	CZ	ARG	138	40.016	5.909	43.327	1.00 16.26	В
	MOTA	973	NH1	ARG	138	39.446	5.743	42.137	1.00 15.29	. В
	ATOM	974		ARG	138	41.337	6.004	43.433	1.00 14.85	В
	MOTA	975	Ç	ARG	138	33.630	8.705	44.202	1.00 21.32	В
15	ATOM ATOM	976 977	N O	ARG THR	138 139	33.021 33.009	8.644 8.667	43.139 45.370	1.00 25.00	B B
13	MOTA	978	ÇA	THR	139	31.562	8.540	45.436	1.00 20.40 1.00 20.86	В
	MOTA	979	CB	THR	139	31.081	8.385	46.895	1.00 20.11	· в
	ATOM	980		THR	139	31.770	7.293	47.512	1.00 21.18	В
	MOTA	981	CG2	THR	139	29.583	8.120	46.944	1.00 18.68	В
20	ATOM	982	С	THR	139	30.883	9.753	44.815	1.00 23.10	В
	ATOM	983	0	THR	139	29.955	9.613	44.014	1.00 24.95	В
	ATOM .	984	N	LEU	140	31.340	10.944	45.189		В
	ATOM	985	CA	LEU	140	30.762	12.175	44.659	1.00 23.38	В
25	MOTA MOTA	986 987	CB CG	LEU	140	31.480 31.211	13.401	45.238	1.00 21.47	В
23	MOTA	988		LEU	140 140	32.120	13.560 14.621	46.733 47.305	1.00 21.91 1.00 21.37	. B
	ATOM	989		LEU	140	29.740	13.883	46.966	1.00 18.69	. В
	ATOM	990	c	LEU	140	30.859	12.184	43.154	1.00 23.10	В
	ATOM	991	0	LEU	140	29.870	12.395	42.467	1.00 21.86	В
30	ATOM	992	N	HIS	141	32.058	11.948	42.645	1.00 24.02	В
	MOTA	993	ÇA	HIS	141	32.272	11.927	41.207	1.00 27.46	В
	MOTA	994	CB	HIS	141	33.741	11.616	40.908	1.00 27.50	В
	MOTA	995	CG	HIS	141	34.101	11.718	39.457	1.00 30.18	В
35	MOTA MOTA	996 997		HIS	141 141	34.041 34.614	10.807 12.869	38.457 38.896	1.00 30.98	B B
55	MOTA	998		HIS	141	34.859	12.662	37.615	1.00 30.79	В
	ATOM	999		HIS	141	34.520	11.419	37.324	1.00 31.87	В
	ATOM	1000	C	HIS	141	31.372	10.885	40.517	1.00 28.79	В
40	MOTA	1001	0	HIS	141	30.835	11.133	39.432	1.00 30.63	В
40	MOTA	1002	N	GLN	142	31.196	9.728	41.154	1.00 27.09	В
	ATOM	1003	CA	GLN	142	30.392	8.664	40.579	1.00 26.11	В
	ATOM	1004	CB	GLN	142	30.660	7.381	41.302	1.00 27.58	В
	MOTA MOTA	1005 1006	CD	GLN GLN	142	31.938	6.733	40.855	1.00 29.72	В
45	MOTA	1005		GLN	142 142	32.001 31.181	6.617 5.929	39.344 38.729	1.00 31.15	B B
	MOTA	1008	NE2	GLN	142	32.969	7.300	38.735	1.00 29.44	В
	ATOM	1009	C	GLN	142	28.894	8.913	40.514	1.00 25.79	В
	MOTA	1010	0	GLN	142	28.238	8.494	39.564	1.00 25.19	В
50	MOTA	1011	N	ILE	143	28.351	9.583	41.523	1.00 24.49	В
50	ATOM	1012	CA	ILE	143	26.928	9.888	41.555	1.00 23.07	В
	MOTA	1013	CB	ILE	143	26.581	10.716	42.805	1.00 22.41	В
	ATOM ATOM	1014 1015		ILE	143 143	25.174 26.727	11.285 9.856	42.690 44.044	1.00 24.89	B B
	ATOM	1016		ILE	143	26.477	10.599	45.339	1.00 21.77	В
55	MOTA	1017	c	ILE	143	26.492	10.664	40.308	1.00 23.84	В
	ATOM	1018	0	ILE	143	25.417	10.425	39.769	1.00 23.49	В
	ATOM	1019	N	PHE	144	27.334	11.593	39.860	1.00 25.75	В
•	MOTA	1020	CA	PHE	144	27.044	12.418	38.690	1.00 27.59	В
4٥	MOTA	1021	CB	PHE	144	28.019	13.657	38.638	1.00 26.93	В
60	MOTA	1022	CG	PHE	144	27.734	14.694	39.688	1.00 27.63	В
	ATOM	1023		PHE	144	26.583	15.478	39.614	1.00 28.58	В
	ATOM ATOM	1024 1025	CD2 CE1		144 144	28.577 26.271	14.845 16.396	40.785 40.626	1.00 27.80 1.00 28.69	B
	ATOM	1025		PHE	144	28.279	15.756	41.802	1.00 28.69	B B
65	ATOM	1027	CZ	PHE	144	27.121	16.532	41.723	1.00 29.86	В
	ATOM	1028	c	PHE	144	27.129	11.621	37.394	1.00 28.56	В
	MOTA	1029	0	PHE	144	26.425	11.918	36.423	1.00 27.83	В
	MOTA	1030	N	GLU	145	27.998	10.614	37.382	1.00 30.60	В
70	ATOM	1031	CA	GLU	145	28.160	9.757	36.209	1.00 32.75	В
/0	ATOM	1032	CB	GLU	145	29.433	8.889	36.357	1.00 35.85	В
	ATOM ATOM	1033 1034	CG CD	GLU	145 145	30.742 31.201	9.673 9.977	36.317 34.898	1.00 42.03	B B
	ATOM	1035		GLU	145	32.014	10.916	34.699	1.00 45.35	B
										_

	MOTA	1036	OE2	GLU	145	30.748	9.262	33.976	1.00 49.72	В
	ATOM	1037	C	GLU	145	26.934	8.854	36.040	1.00 32.32	В
	MOTA	1038	0	GLU	145	26.319	8.812	34,974	1.00 32.21	В
	MOTA	1039	N	LYS	146	26.573	8.150	37.104	1.00 31.79	В
5	ATOM	1040	CA	LYS	146	25.443	7.235	37.066	1.00 34.10	В
5										
	ATOM	1041	CB	LYS	146	25.340	6.463	38.430	1.00 34.57	В
	ATOM	1042	CG	LYS	146	26.693	5.973	38.952	1.00 35.68	В
	MOTA	1043	CD	LYS	146	26.597	4.862	39.994	1.00 34.50	В
10	MOTA	1044	CE	LYS	146	26.566	3.486	39.327	1.00 35.54	В
10	MOTA	1045	NZ	LYS	146	27.115	2.405	40.204	1.00 33.09	В
	ATOM	1046	C	LYS	146	24.098	7.888	36.721	1.00 34.95	В
						23.320	7.342	35.929	1.00 35.60	В
	MOTA	1047	0	LYS	146					
	MOTA	1048	N	LEU	147	23.831	9.057	37.298	1.00 34.40	В
	MOTA	1049	CA	LEU	147	22.574	9.762	37.061	1.00 33.66	В
15	MOTA	1050	CB	LEU	147		10.477	38.336	1.00 32.95	В
13										
	MOTA	1051	CG	LEU	147	21.963	9.607	39.554	1.00 33.64	В
	MOTA	1052	CD1	LEU	147	21.682	10.474	40.775	1.00 34.40	В
	MOTA	1053	CD2	LEU	147	20.809	8.645	39.308	1.00 35.51	В
							10.772			B
20	MOTA	1054	Ç	LEU	147	22.634		35.907	1.00 34.15	
20	MOTA	1055	0	LEU	147	21.724	11.576	35.728	1.00 32.96	, B
	ATOM	1056	N	THR	148	23.698	10.719	35.115	1.00 35.64	В
	MOTA	1057	CA	THR	148	23.863	11.656	34.011	1.00 36.46	В
	MOTA	1058	CB	THR	148	25.138	11.332	33.198	1.00 35.78	В
	MOTA	1059	0G1	THR	148	25.492	12.468	32.409	1.00 36.67	·B
25	ATOM	1060	CG2	THR	148	24.914	10.150	32.274	1.00 36.63	В
						22.659				В
	ATOM	1061	C	THR	148		11.770	33.057	1.00 37.44	
	MOTA	1062	0	THR	148	22.313	12.878	32.639	1.00 37.93	В
	ATOM	1063	N	ASP	149	22:019	10.653	32.712	1.00 35.78	В
	MOTA	1064	CA	ASP	149	20.867	10.706	31.807	1.00 35.94	. в
30										
20	MOTA	1065	CB	ASP	149	21.337	11.004	30.322	1.00 34.77	В
	ATOM	1066	CG	ASP	149	22.404	10.027	29.827	1.00 36.65	В
	MOTA	1067	OD1	ASP	149	22.605	8.965	30.467	1.00 35.17	В
	MOTA	1068		ASP	149	23.032	10.321	28.784	1.00 35.41	В
05.	MOTA	1069	С	ASP	149	19.966	9.460	31.824	1.00 36.15	В
35 ·	MOTA	1070	0	ASP	149	19.568	8.947	30.769	1.00 32.78	В
	MOTA	1071	N	ASN	150	19.639	8.987	33.025	1.00 36.51	В
	MOTA	1072	CA	asn	150	18.781	7.819	33.181	1.00 38.16	В
	MOTA	1073	CB	ASN	150	19.218	6.992	34.417	1.00 37.97	В
	MOTA	1074	CG	ASN	150	19.159	7.785	35.704	1.00 37.13	В.
40	MOTA	1075		ASN	150	19.548	8.951	35.742	1.00 37.20	В
70										
	MOTA	1076	NDZ	ASN	150	18.694	7.148	36.774	1.00 36.82	В
	MOTA	1077	С	ASN	150	17.314	8.240	33.305	1.00 39.47	В
	MOTA	1078	0	ASN	150	16.419	7397	33.433	1.00 39.49	В
	ATOM	1079	N	GLY	151	17.077	9.549	33.245	1.00 39.29	В
45										
43	MOTA	1080	CA	GLY	151	15.725	10.063	33.343	1.00 39.01	В
	ATOM	1081	С	GLY	151	15.333	10.349	34.772	1.00 39.23	В
	MOTA	1082	Ο.	GLY	151	14.170	10.612	35.063	1.00 40.53	В
										В
	MOTA	1083	N	THR	152	16.307	10.285	35.670	1.00 40.25	
5 0	MOTA	1084	CA	THR	152	16.069	10.547	37.085	1.00 40.87	В
50	MOTA	1085	CB	THR	152	16.730	9.463	37.960	1.00 39.78	В
	MOTA	1086	OG1	THR	152	16.146	8.191	37.655	1.00 43.27	В
	MOTA	1087		THR	152	16.531	9.764	39.437	1.00 40.09	В
	MOTA	1088	С	THR	152	16.643	11.918	37.448	1.00 41.24	В
	MOTA	1089	0	THR	152	17.860	12.120	37.434	1.00 42.84	В
55	MOTA	1090	N	GLU	153	15.753	12.856	37.754	1.00 40.50	В
	ATOM		CA					38.118	1.00 39.45	В
		1091		GLU	153	16.140	14.216			
	MOTA	1092	СВ	GLU	153	14.910	15.143	38.054	1.00 41.77	В
	ATOM	1093	CG	GLU	153	15.258	16.606	37.831	1.00 47.08	В
	MOTA	1094	CD	GLU	153	15.903	16.847	36.474	1.00 49.24	В
60 ·										
00	MOTA	1095		GLU	153	16.559	17.901	36.313	1.00 49.10	В
	MOTA	1096	OE2	GLU	153	15.747	15.988	35.570	1.00 49.10	В
	MOTA	1097	С	GLU-	153	16.697	14.170	39.538	1.00 36.82	В
	ATOM	1098	ō	GLU	153	16.140	13.472	40.387	1.00 35.59	В
CE	ATOM	1099	N	PHE	154	17.770	14.919	39.807	1.00 33.77	В
65	ATOM	1100	CA	PHE	154	18.380	14.877	41.140	1.00 31.58	В
	MOTA	1101	CB	PHE	154	19.302	13.644	41.212	1.00 29.10	В
	ATOM	1102	CG	PHE	154	20.572	13.797	40.414	1.00 25.93	В
	MOTA	1103	CD1	PHE	154	21.763	14.165	41.038	1.00 25.72	В
	ATOM	1104	CD2	PHE	154	20.573	13.597	39.037	1.00 23.66	В
70	MOTA	1105		PHE	154	22.941	14.328	40.297	1.00 26.03	В
, •										
	MOTA	1106	CE2		154	21.741	13.758	38.294	1.00 25.52	В
	MOTA	1107	CZ.	PHE	154	22.930	14.123	38.925	1.00 24.44	В
	MOTA	1108	C	PHE	154	19.183	16.093	41.627	1.00 29.93	В
			-							_

	MOTA	1109	0	PHE	154	19.651	16.924	40.850	1.00 30.00	₿
	MOTA	1110	N	SER	155	19.357	16.157	42.940	1.00 28.97	В
	MOTA	1111	CA	SER	155	20.140	17.212	43.572	1.00 28.90	В
-	MOTA	1112	CB	SER	155	19.225	18.281	44.243	1.00 26.53	В
5	MOTA	1113	OG	SER	155	18.732	17.844	45.502	1.00 24.48	В
	MOTA	1114	С	SER	155	21.010	16.537	44.635	1.00 28.97	В
	MOTA	1115	0	SER	155	20.588	15.569	45.279	1.00 28.86	В
	MOTA	1116	N	VAL	156	22.221	17.047	44.819	1.00 29.35	В
10	MOTA	1117	CA	VAL	156	23.135		45.803	1.00 29.64	В
10	ATOM	1118	CB	VAL	156	24.431	15.977	45.125	1.00 28.79	В
	MOTA	1119	CG1		156	25.280	15.208	46.124	1.00 29.92	• В
	ATOM	1120		VAL	156	24.089	15.116	43.930	1.00 29.12	В
	MOTA	1121	C	VAL	156	23.516	17.517	46.863	1.00 29.76	В
15	ATOM	1122	0	VAL	156	23.925	18.627	46.532	1.00 30.11	В
13	ATOM	1123	N	LYS	157	23.372	17.149	48.132	1.00 30.23	В
	MOTA	1124	CA	LYS	157	23.731	18.028	49.245	1.00 31.02	В
	ATOM	1125	CB	LYS	157	22.489	18.431	50.063	1.00 32.19	В
	ATOM	1126	CG	LYS	157	21.543	19.376	49.364 50.162	1.00 35.38	В
20	MOTA MOTA	1127 1128	CD	LYS	157 157	20.246 19.169	19.523 20.259	49.369	1.00 39.38	B B
20	ATOM	1129	NZ	LYS	157	17.857	20.233	50.067	1.00 40.45	В
	ATOM .	1130	C	LYS	157	24.702	17.308	50.171	1.00 30.04	В
	ATOM	1131	ŏ	LYS	157	24.399	16.230	50.668	1.00 30.82	В
	ATOM	1132	N	VAL	158	25.866	17.900	50.402	1.00 30.82	В
25	ATOM	1133	CA	VAL	158	26.839	17.290	51.292	1.00 27.63	• В
	ATOM	1134	CB	VAL	158	28.284	17.406	50.751	1.00 27.29	В
	ATOM	1135		VAL	158	28.433	16.582	49.478	1.00 29.26	В
	MOTA	1136	CG2		158	28.632	18.861	50.491	1.00 26.29	В
	ATOM	1137	c	VAL	158	26.785	17.959	52.649	1.00 27.62	В
30	ATOM	1138	ō	VAL	158	26.182	19.009	52.818	1.00 27.51	В
	ATOM	1139	N	SER	159	27.431	17.344	53.624	1.00 28.77	В
	ATOM	1140	CA	SER	159	27.449	17.896	54.962	1.00 29.25	В
	MOTA	1141	CB	SER	159.	26.155	17.634	55.612	1.00 29.36	В
	MOTA	1142	OG	SER	159	26.083	18.324	56.835	1.00 35.64	В
35	MOTA	1143	С	SER	159	28.584	17.255	55.753	1.00 28.48	В
	MOTA	1144	0	SER	159	28.762	16.037	55.723	1.00 29.46	В
	MOTA	1145	N	LEU	160	29.364	18.070	56.451	1.00 26.66	В
	MOTA	1146	CA	LEU	160	30.473	17.529	57.215	1.00 26.24	В
40	MOTA	1147	CB	LEU	160	31.769	18.008	56.649	1.00 26.22	В
40	MOTA	1148	CG	LEU	160	33.024	17.381	57.255	1.00 25.56	B
	MOTA	1149		LEU	160	32.850	15.873	57.350	1.00 24.56	В
	MOTA	1150		LEU	160	34.241	17.759	56.400	1.00 24.75	В
	ATOM	1151	С	LEU	160	30.393	17.872	58.690	1.00 26.51	В
15	MOTA	1152	0	LEU	160	30.816	18.949	59.119	1.00 24.86	В
45	ATOM	1153	N	LEU	161	29.844	16.937	59.461	1.00 25.32	В
	MOTA	1154	CA	LEU	161	29.686	17.112	60.895	1.00 23.81	В
	MOTA	1155	CB	LEU	161	28.349	16.607	61.310	1.00 23.24	В
	MOTA	1156	CG	LEU	161	28.109	16.490	62.766	1.00 23.19	В
50	MOTA MOTA	1157 1158		LEU	161	27.992	17.879 15.701	63.371	1.00 24.82	В
50	MOTA	1159	CD2	LEU LEU	161 161	26.838 30.777		62.989	1.00 22.84	B B
	MOTA	1160	ŏ	LEU	161	31.024	16.338 15.178	61.613 61.307	1.00 25.43	В
	MOTA	1161	N	GLU	162	31.444	16.983	62.563	1.00 23.56	В
	MOTA	1162	CA	GLU	162	32.507	16.322	63.304	1.00 21.29	В
55	MOTA	1163	СВ	GLU	162	33.892	16.895	62.872	1.00 19.65	В
-	MOTA	1164	CG	GLU	162	34.027	16.956	61.338	1.00 18.31	В
	ATOM	1165	CD	GLU	162	35.463	16.923	60.845	1.00 19.90	В
	MOTA	1166		GLU	162	36.362	17.416	61.557	1.00 20.88	В
	MOTA	1167		GLU	162	35.699	16.413	59.729	1.00 21.08	В
60	ATOM	1168	C	GLU	162	32.276	16.448	64.803	1.00 21.51	В
	MOTA	1169	ŏ	GLU	162	31.734	17.441	65.286	1.00 24.11	В
	MOTA	1170	N	ILE	163	32.665	15.419	65.543	1.00 20.50	В
	MOTA	1171	CA	ILE	163	32.464	15.414	66.979	1.00 16.52	В
	ATOM	1172	СВ	ILE	163	31.587	14.221	67.396	1.00 15.68	В
65	ATOM	1173		ILE	163	31.070	14.412	68.813	1.00 13.11	В
	ATOM	1174		ILE	163	30.420	14.093	66.427	1.00 14.88	В
	ATOM	1175		ILE	163	29.521	12.920	66.704	1.00 16.15	В
	ATOM .	1176	C	ILE	163	33.805	15.325	67.672	1.00 17.43	В
	ATOM	1177	ō	ILE	163	34.644	14.499	67.319	1.00 17.59	В
70	MOTA	1178	N	TYR	164	33.996	16.201	68.654	1.00 17.46	В
	MOTA	1179	CA	TYR	164	35.219	16:263	69.430	1.00 16.57	В
	MOTA	1180	СВ	TYR	164	36.192	17.276	68.783	1.00 14.70	В
	MOTA	1181	CG	TYR	164	37.464	17.474	69.559	1.00 12.25	В

	MOTA	1182	CD1	TYR	164	37.502	18:334	70.653	1.00 13.17	. в
	MOTA	1183	CE1	TYR	164	38.643	18.439	71.454	1.00 15.94	В
	MOTA	1184	CD2	TYR	164	38.600	16.724	69.267	1.00 13.00	В
		1185		TYR	164					
5	MOTA		CE2			39.753	16.814	70.058	1.00 15.22	В
,	MOTA	1186	CZ	TYR	164	39.773	17.674	71.155	1.00 17.31	В
	MOTA	1187	ОН	TYR	164	40.909	17.774	71.952	1.00 15.71	В
	MOTA	1188	С	TYR	164	34.875	16.669	70.863	1.00 18.56	В
	MOTA	1189	0	TYR	164	34.289	17.726	71.094	1.00 21.94	В
	MOTA	1190	N	ASN	165	35.225	15.826	71.828	1.00 20.33	В
10	ATOM	1191	CA	ASN	165	34.942	16.122	73.232	1.00 22.94	В
~~										
	MOTA	1192	·CB	ASN	165	35.633	17.402	73.653	1.00 24.28	В
	ATOM	1193	CG	ASN	165	36.418	17.255	74.942	1.00 28.53	В
	ATOM	1194	OD1	ASN	165	37.598	16.864	74.929	1.00 31.28	В
	ATOM	1195	ND2	ASN	165	35.777	17.569	76.064	1.00 24.86	В
15	MOTA	1196	С	ASN	165	33.443	16.314	73.406	1.00 24.90	В
	MOTA	1197	Ō	ASN	165	33.009	17.222	74.121	1.00 26.77	В
•	ATOM	1198	N	GLU	166	32.657	15.471	72.745		B
									1.00 23.40	
	ATOM	1199	CA	GLU	166	31.200	15.555	72.813	1.00 22.69	В
20	MOTA	1200	CB	GLU	166	30.706	15.231	74.237	1.00 22.07	В
20	MOTA	1201	CG	GLU	166	30.814	13.757	74.590	1.00 22.71	. в
	MOTA	1202	CD	GLU	166	30.157	12.849	73.548	1.00 23.19	В
	MOTA	1203	OE1	GLU	166	28.906	12.779	73.505	1.00 22.44	В.
	ATOM	1204	OE2	GLU	166	30.899	12.211	72.769	1.00 21.71	В
	ATOM	1205	C	GLU	166	30.610	16.884	72.349	1.00 22.21	·B
25	ATOM	1206		GLU		29.491				
23			0		166		17.228	72.709	1.00 22.53	В
	MOTA	1207	N	GLU	167	31.363	17.631	71.545	1.00 24.18	B
	MOTA	1208	CA	GLU	167	30.885	18.899	71.011	1.00 23.58	В
	MOTA	1209	CB	GLU	167	31.825	20.009	71.365	1.00 28.43	В
	MOTA	1210	CG	GLU	167	31.900	20.321	72.848	1.00 34.21	В
30	MOTA	1211	CD	GLU	167	32.857	21.470	73.142	1.00 40.07	В
	MOTA	1212	OE1	GLU	167	34.033	21.400	72.702	1.00 41.07	В
	ATOM	1213	OE2	GLU	167	32.431	22.441	73.812	1.00 43.47	B
•	ATOM	1214	C	GLU	167					
						30.800	18.766	69.500	1.00 22.74	В
35	ATOM	1215	0	GLU	167	31.659	18.142	68.884	1.00 23.08	В
22	ATOM	1216	N	LEU	168	29.766	19.347	68.904	1.00 21.20	В
	ATOM	1217	CA	LEU	168	29.578	19.274	67.461	1.00 20.52	В
	MOTA	1218	CB	LEU	168	28.088	19.156	67.125	1.00 21.09	В
	ATOM	1219	CG	LEU	168	27.319	17.889	67.681	1.00 22.11	В
	ATOM	1220		LEU	168	28.249	16.663	67.622	1.00 15.69	В
40	ATOM	1221		LEU	168	26.837	18.136	69.114		
									1.00 21.13	В
	ATOM	1222	C	LEU	168	30.173	20.458	66.702	1.00 21.77	В
	MOTA.	1223	Ó	LEU	168	30.178	21.598	67.179	1.00 22.45	В
	ATOM	1224	N	PHE	169	30.673	20.171	65.506	1.00 20.28	В
4.5	MOTA	1225	CA	PHE	169	31.282	21.180	64.665	1.00 19.17	В
45	MOTA	1226	CB	PHE	169	32.835	21.112	64.778	1.00 19.31	В
	MOTA	1227	CG	PHE	169	33.345	21.308	66.177	1.00 19.18	В
	MOTA	1228		PHE	169	33.688	20.213	66.966	1.00 20.05	В
	MOTA	1229		PHE	169	33.434	22.591	66.722	1.00 18.70	В
	ATOM	1230		PHE						
50					169	34.112	20.385	68.281	1.00 19.61	В
50	MOTA	1231		PHE	169	33.852	22.782	68.027	1.00 18.44	В
	MOTA	1232	CZ	PHE	169	34.193	21.676	68.814	1.00 22.70	В
	MOTA	1233	С	PHE	169	 30.865	20.981	63.220	1.00 20.25	В
	MOTA	1234	0	PHE	169	30.476	19.880	62.808	1.00 20.20	В
	MOTA	1235	N	ASP	170	30.949	22.064	62.462	1.00 19.31	В
55	ATOM	1236	CA	ASP	170	30.603	22.069	61.053	1.00 19.06	В
	ATOM	1237	СВ	ASP	170	29.549	23.141	60.785	1.00 19.49	13
		1238	CG							
	MOTA			ASP	170	28.970	23.066	59.386	1.00 21.37	В
	MOTA	1239		ASP	170	29.648	22.556	58.463	1.00 20.46	₿.
~	MOTA	1240	OD2	ASP	170	27.827	23.542	59.206	1.00 24.10	В
60 ·	ATOM	1241	C .	ASP	170	31.902	22.429	60.353	1.00 20.21	В
	ATOM	1242	0	ASP	170	32.402	23.540	60.509	1.00 21.52	В
	MOTA	1243	N	LEU	171	32.460	21.492	59.599	1.00 20.15	В
	ATOM	1244	CA	LEU	171	33.699			1.00 22.53	
		1245					21.758	.58.900		В
65	ATOM		CB	LEU	171	34.620	20.517	58.965	1.00 19.76	В
O)	ATOM	1246	CG	LEU	171	35.385	20.297	60.340	1.00 18.93	В
	MOTA	1247		LEU	171	36.562	21.251	60.487	1.00 16.80	В
	MOTA	1248	CD2	LEU	171	34.426	20.479	61.495	1.00 18.41	В
	MOTA	1249	С	LEU	171	33.460	22.198	57.459	1.00 24.95	В
	MOTA	1250	ō	LEU	171	34.374	22.169	56.632	1.00 25.06	В
70	MOTA	1251	N	LEU	172	32.233	22.618	57.160	1.00 28.25	
	MOTA				172					В
		1252	CA	LEU		31.910	23.081	55.812	1.00 33.55	В
	ATOM	1253	CB	LEU	172	31.001	22.111	55.116	1.00 33.77	В
	MOTA	1254	CG	LEU	172	31.664	20.867	54.556	1.00 34.20	В

	ATOM	1255	CD1	LEU	172	30.632	20.056	53.783	1.00 33.48	В
	ATOM	1256		LEU	172	32.807	21.268	53.644	1.00 34.44	B
	MOTA	1257	C.	LEU	172	31.279	24.461	55.766	1.00 35.97	В
_	MOTA	1258	0	LEU	172	31.181	25.059	54.706	1.00 37.85	В
5	MOTA	1259	N	ASN	173	30.843	24.962	56.912	1.00 39.07	В
-										
	MOTA	1260	CA.	ASN	173	30.242	26.284	56.972	1.00 44.33	В
	MOTA	1261	CB	ASN	173	29.451	26.445	58.275	1.00 45.10	В
	MOTA	1262	CG	ASN	173	28.700	27.765	58.345	1.00 47.21	В
		1263		ASN	173		27.987	59.254	1.00 46.55	
10	MOTA									В
10	MOTA	1264	ND2	asn	173	28.958	28.650	57.384	1.00 47.66	В
	ATOM	1265	С	ASN	173	31.355	27.330	56.903	1.00 48.18	В
	ATOM	1266	ō	ASN	173	32.094	27.532	57.871	1.00 47.58	В
	MOTA	1267	N	PRO	174	31.492	28.007	55.752	1.00 51.96	В
	MOTA	1268	CD	PRO	174	30.737	27.802	54.502	1.00 52.92	В
15	MOTA	1269	CA	PRO	174 -	32.527	29.030	55.572	1.00 55.50	В
	ATOM	1270	CB	PRO	174	32.609	29.162	54.076	1.00 54.73	В
	MOTA	1271	CG	PRO	174	31.184	28.973	53.660	1.00 53.60	В
•	ATOM	1272	С	PRO	174	32.226	30.364	56.259	1.00 58.47	В
	MOTA	1273	0	PRO	174	33.076	31.256	56.286	1.00 59.03	В
20										
20	MOTA	1274	N	SER	175	31.024	30.497	56.819	1.00 60.76	В
	ATOM	1275	CA	SER	175	30.639	31.730	57.504	1.00 62.73	В
	ATOM	1276	CB	SER	175	29.138	32.013	57.301	1.00 63.76	В
	MOTA	1277	OG	SER	175	28.877	32.450	55.975	1.00 66.00	В
25	MOTA	1278	С	SER	175	30.957	31.725	59.000	1.00 63.50	В
25	ATOM	1279	0	SER	175	30.901	32.769	59.654	1.00 63.94	· B
	ATOM	1280	N	SER	176	31.293	30.557	59.543	1.00 63.63	. в
	ATOM	1281	CA	SER	176	31.613	30.456	60.964	1.00 63.17	В
	MOTA	1282	CB	SER	176	30.589	29.549	61.694	1.00 63.04	В
	MOTA	1283	OG	SER	176	30.805	28.181	61.389	1.00 64.15	В
30	MOTA	1284	С	SER	176	33.017	29.909	61.188	1.00 62.90	В
	ATOM	1285	ŏ	SER	176	33.758	29.643	60.238	1.00 62.07	
			-							В
	ATOM	1206	N	ASP	177	33.371	29.744	62.459	1.00 62.85	В
	MOTA	1287	CA	ASP	177	34.676	29.225	62.837	1.00 62.62	В
	ATOM	1288	CB	ASP	177	35.352	30.147	63.856	1.00 63.20	В
35	MOTA	1289	CG	ASP	177	35.504			1.00 63.21	В.
JJ							31.559	63.345		
	ATOM	1290	OD1		177	36.062	31.729	62.243	1.00 63.09	В
	MOTA	1291	OD2	ASP	177	35.068	32.498	64.044	1.00 62.91	В
	ATOM	1292	С	ASP	177	34.515	27.852	63.452	1.00 61.87	В
	ATOM	1293	ŏ	ASP	177	33.447	27.504			
40								63.954	1.00 62.79	В
40	ATOM	1294	N	VAL	178	35.588	27.078	63.415	1.00 60.45	В
	ATOM	1295	CA	VAL	178	35.572	25.743	63.977	1.00 59.51	В
	MOTA	1296	CB	VAL	178	36.894	25.005	63.688	1.00 59.52	В
	ATOM	1297	CG1		178	37.118	24.909	62.183	1.00 59.92	В
45	MOTA	1298	CG2		178	38.048	25.729	64.356	1.00 59.97	В
45	ATOM	1299	С	VAL	178	35.363	25.834	65.485	1.00 58.12	В
	ATOM	1300	0	VAL	178	35.159	24.825	66.157	1.00 59.80	В
	ATOM	1301	N	SER	179	35.421	27.047	66.016	1.00 55.31	В
	MOTA	1302	CA	SER	179	35.221	27.245	67.443	1.00 52.98	В
	ATOM	1303	СB	SER	179	35.823	28.578	67.871	1.00 51.75	В
50	ATOM	1304	OG	SER	179	35.401	29.619	67.011	1.00 50.71	В
	ATOM	1305	С	SER	179	33.725	27.211	67.746	1.00 52.04	В
					179			68.860		
	ATOM	1306	0	SER		33.313	26.894		1.00 52.07	В
	MOTA	1307	N	GLU	180	32.917	27.535	66.743	1.00 51.08	В
	MOTA	1308	CA	GLU	180	31.467	27.541	66.882	1.00 50.67	В
55	MOTA	1309	CB	GLU	180	30.834	28.188	65.639	1.00 53.74	В
-										
	MOTA	1310	CG	GLU	180	29.322	28.334	65.691	1.00 57.88	В
	ATOM	1311	CD	GLU	180	28.872	29.401	66.666	1.00 60.00	В
	MOTA	1312	OE1	GLU	180	29.192	29.279	67.868	1.00 61.89	В
	ATOM	1313	OE2		180	28.199	30.362	66.230	1.00 61.08	В
60										
00	ATOM	1314	C	GLU	180	30.989	26.096	67.026	1.00 48.91	В
	MOTA	1315	0	GLU	180	31.307	25.249	66.196	1.00 49.20	В
	MOTA	1316	N	ARG	181	30.234	25.817	68.082	1.00 46.31	В
	ATOM	1317	CA	ARG	181	29.739	24.472	68.332	1.00 44.31	В
						30.194				
45	MOTA	1318	CB	ARG	181		24.018	69.710	1.00 46.69	В
65	MOTA	1319	CG	ARG	181	29.815	24.962	70.842	1.00 50.74	В
	ATOM	1320	CD	ARG '	181	28.527	24.530	71.547	1.00 55.78	В
	ATOM	1321	NE	ARG	181	28.677	23.242	72.234	1.00 60.23	В
	MOTA	1322	CZ	ARG	181	27.708	22.628	72.913	1.00 61.32	В
	MOTA	1323	NH1		181	26.501	23.180	73.007	1.00 61.66	В
70	ATOM	1324	NH2	ARG	181	27.945	21.453	73.490	1.00 61.67	В
	ATOM	1325	С	ARG	181	28.217	24.395	68.211	1.00 42.65	В
	MOTA	1326	0	ARG	181	27.491	25.115	68.888	1.00 42.59	В
	ATOM	1327	N	LEU	182	27.739	23.510	67.344	1.00 39.35	В

	АТОМ	1328	CA	LEU	182	26.310	23:355	67.110	1.00 35.22	В
	MOTA	1329	CB	LEU	182	26.088	22.559	65.843	1.00 32.83	В
	ATOM	1330	CG	LEU	182	26.998	22.979	64.710	1.00 31.23	В
5	ATOM	1331		LEU	182	26.730	22.114	63.508	1.00 32.55	В
)	ATOM	1332		LEU	182	26.776	24.444	64.386	1.00 31.45	В
	MOTA MOTA	1333	C	LEU	182	25.581	22.690	68.260	1.00 33.98	В
	ATOM	1334 1335	O N	LEU GLN	182 183	26.197 24.259	22.057 22.843	69.117 68.266	1.00 33.33	B B
	ATOM	1336	CA	GLN	183	23.399	22.259	69.296	1.00 33.20	В
10	MOTA	1337	СВ	GLN	183	22.430	23.320	69.842	1.00 34.22	В
	ATOM	1338	·CG	GLN	183	23.122	24.542	70.436	1.00 37.39	В
	MOTA	1339	CD	GLN	183	22.163	25.699	70.671	1.00 38.77	В
	MOTA	1340	OE1	GLN	183	21.325	26.003	69.818	1.00 39.62	В
1.5	MOTA	1341	NE2	GLN	183	22.294	26,361	71, 820	1.00 37.72	В
15	ATOM	1342	C	GLN	183	22.603	21.099	68.706	1.00 31.57	В
	ATOM	1343	0	GLN	183	22.209	21.134	67.545	1.00 31.18	В
	MOTA	1344	N	MET	184	22.353	20.079	69.513	1.00 31.59	В
	MOTA ATOM	1345 1346	CA CB	MET	184 184	21.622 22.480	18.908 17.677	69.052	1.00 32.44	В
20	ATOM	1347	CG	MET	184	22.018	16.404	69.297 68.626	1.00 32.63 1.00 34.09	B B
	ATOM	1348	SD	MET	184	23.162	15.016	68.908	1.00 32.00	В
	ATOM	1349	CE	MET	184	22.574	14.436	70.488	1.00 31.68	B .
	MOTA	1350	C	MET	184	20.289	18.787	69.791	1.00 34.68	B
~~	MOTA	1351	0	MET	184	20.203	19.114	70.976	1.00 35.18	·B
25	MOTA	1352	N	PHE	185	19.248	18.345	69.086	1.00 36.66	В
	MOTA	1353	CA	PHE	185	17.922	18.168	69.690	1.00 39.01	B _.
	MOTA	1354	CB	PHE	185	16.987	19.422	69.462	1.00 37.84	, В
	ATOM	1355	CG	PHE	185	17.676	20.750	69.619	1.00 38.18	В
30	ATOM ATOM	1356 1357		PHE	185 185	18.453 17.534	21.270	68.593 70.793	1.00 36.50	В
50	ATOM	1358		PHE	185	19.080	21.488 22.502	68.724	1.00 38.31 1.00 36.83	B B
	MOTA	1359		PHE	185	18.158	22.724	70.936	1.00 38.32	В
•	ATOM	1360	cz	PHE	185	18.933	23.232	69.897	1.00 38.06	В
	MOTA	1361	C	PHE	185	17.224	16:956	69.077	1.00 40.70	В
35 °	MOTA	1362	0	PHE	185	17.485	16.598	67.931	1.00 39.58	В
٠	MOTA	1363	N	ASP	186	16.333	16.330	69.838	1.00 43.77	В
	ATOM	1364	CA	ASP	186	15.588	15.187	69.328	1.00 46.67	В
	MOTA	1365	CB	ASP	186		14.550	70.419	1.00 47.89	В
40	MOTA	1366	CG	ASP	186	15.534	14.206	71.659	1.00 50.45	В
40	MOTA	1367		ASP	186	16.535	13.461	71.540	1.00 50.63	В
	ATOM ATOM	1368 1369	C	ASP ASP	186 186	15.154 14.668	14.679 15.740	72.756 68.262	1.00 51.23 1.00 47.79	B B
	MOTA	1370	ŏ	ASP	186	14.371	16.933	68.246	1.00 47.79	В
	ATOM	1371	N	ASP	187	14.215	14.883	67.365	1.00 50.77	В
45	ATOM	1372	CA	ASP	187	13.318	15.351	66.328	1.00 54.90	В
	ATOM	1373	CB	ASP	187	13.748	14.832	64.990	1.00 56.93	В
	MOTA	1374	CG	ASP	187	12.973	15.457	63.860	1.00 59.28	В
	MOTA	1375		ASP	187	13.425	15.343	62.700	1.00 60.01	В
50	MOTA	1376		ASP	187	11.910	16.060	64.138	1.00 60.38	В
50	MOTA	1377 1378	c	ASP	187	11.915 11.638	14.877	66.662	1.00 56.34	В
	MOTA MOTA	1379	и О	ASP PRO	187 188	11.015	13.678 15.820	66.649 66.985	1.00 56.08 1.00 58.11	. B
	ATOM	1380	CD	PRO	188	11.251	17.274	66.963	1.00 57.99	. В
	ATOM	1381	CA	PRO	188	9.621	15.529	67.339	1.00 60.11	В
55	MOTA	1382	СВ	PRO	188	8.978	16.890	67.309	1.00 59.76	В
	MOTA	1383	CG	PRO	188	10.091	17.790	67.764	1.00 58.23	В
	MOTA	1384	С	PRO	188	8.956	14.549	66.376	1.00 61.87	В
	MOTA	1385	0	PRO	188	8.162	13.700	66.783	1.00 61.46	В.
٤٥ .	MOTA	1386	N	ARG	189	9.302	14.669	65.100	1.00 64.31	В
60	MOTA	1387	CA.	ARG	189	8:757	13.812	64.058	1.00 66.68	В
	ATOM	1388	CB	ARG	189	9.307	14.265	62.701	1.00 66.61	В
	MOTA MOTA	1389 1390	CG CD	ARG ARG	189 189	8.813 9.586	15.651 16.213	62.277	1.00 66.58 1.00 66.65	В
	MOTA	1391	NE	ARG	189	10.834	16.866	.61.080 61.474	1.00 66.83	B B
65	ATOM	1392	CZ	ARG	189	11.704	17.407	60.625	1.00 66.09	В
	ATOM	1393		ARG	189	11.474	17.377	59.319	1.00 66.33	В
	ATOM	1394		ARG	189	12.803	17.988	61.083	1.00 65.55	В
	ATOM	1395	С	ARG	189	9.041	12.321	64.289	1.00 68.64	В
70	MOTA	1396	0	ARG	189	8.300	11.461	63.813	1.00 69.00	В
70	MOTA	1397	N	ASN	190	10.110	12.018	65.022	1.00 71.07	В
	MOTA	1398	CA	ASN	190	10.487	10.634	65.329	1.00 72.28	В
	ATOM	1399 1400	CB	ASN	190	10.758	9.814	63.998	1.00 72.30	В
	MOTA	1400	CG	ASN	190	11.706	10.525	63.041	1.00 71.90	В

	MOTA	1401	OD1	ASN	190	12.847	10.822	63.385	1.00 71.47	В
	MOTA	1402		ASN	190	11.233	10.789	61.826	1.00 71.27	В
	MOTA	1403		_						
			C.	ASN	190	11.709	10.579	66.252	1.00 73.09	В
_	MOTA	1404	0	ASN	190	12.783		65.905	1.00 73.71	В
5	MOTA	1405	N	LYS	191	11.534	9.979	67.427	1.00 73.58	В
	MOTA	1406	CA	LYS	191	12.601	9.871	68.428	1.00 73.23	В
	MOTA	1407	СВ	LYS	191	12.123	9.021	69.606	1.00 75.05	В
	MOTA	1408	CG	LYS	191	11.285	9.778	70.614	1.00 76.84	В
	MOTA				191			71.241		
10		1409	CD	LYS			10.920		1.00 77.87	В
10	MOTA	1410	CE	LYS	191	11.299	11.547	72.387	1.00 78.94	В
	MOTA	1411	NZ	LYS	191	9.939	11.988	71.961	1.00 79.06	В
	MOTA	1412	С	LYS	191	13.965	9.351	67.968	1.00 71.65	В
	MOTA	1413	0	LYS	191	15.000	9.869	68.395	1.00 71.97	В
	MOTA	1414	N	ARG	192	13.977	8.326	67.121	1.00 68.70	В
15	MOTA	1415	CA	ARG	192	15.238	7.772	66.638	1.00 65.72	В
	MOTA	1416	CB	ARG	192	14.978	6.515	65.768	1.00 67.67	В
	MOTA	1417	CG	ARG	192	16.217	5.978	65.052	1.00 69.51	В
	MOTA	1418	CD	ARG	192	16.068	4.519	64.616	1.00 70.83	В
- A-O'	MOTA	1419	ΝĒ	ARG	192	14:855	4.261	63.839	1.00 71.87	В
20	ATOM	1420	CZ	ARG	192	13.672	3.950	64.364	1.00 71.73	В
	MOTA	1421	NH1	ARG	192	. 13.527	3.855	65.681	1.00 70.61	В
	MOTA	1422		ARG	192	12.631	3.727	63.569	1.00 71.53	В
	ATOM	1423	C	ARG	192	16.033	8.803	65.843	1.00 62.08	В
25	MOTA	1424	0	ARG	192	17.190	8.572	65.482	1.00 61.32	₿
23	MOTA	1425	N	GLY	193	15.403	9.946	65.585	1.00 58.42	• В
	MOTA	1426	CA	GLY	193	16.045	11.008	64.828	1.00 52.07	В
	ATOM	1427	С	GLY	193	16.519	12.171	65.674	1.00 47.14	В
	MOTA	1428	0	GLY	193	16.159	12.300	66.843	1.00 46.94	В
	MOTA	1429	N	VAL	194	17.323	13.033	65.067	1.00 44.16	В
30	MOTA	1430	CA	VAL	194	17.875	14.184	65.757	1.00 40.67	
50						-				В
	MOTA	1431	CB	VAL	194	19.266	13.838	66.329	1.00 39.96	В
	MOTA	1432		VAL	194	20.338	14.058	65.271	1.00 37.96	В
	MOTA	1433	CG2	VAL	194	19.539	14.653	67.564	1.00 39.63	В
	MOTA	1434	С	VAL	194	18.008	15.373	64.800	1.00 39.90	В
35	MOTA	1435	0	VAL	194	18.145	15.194	63.592	1.00 40.91	В
	MOTA	1436	N	ILE	195	17.965	16.585	65.347	1.00 38.55	В
	MOTA	1437	CA	ILE	195	18.104				
							17.803	64.553	1.00 35.81	В
	MOTA	1438	CB	ILE	195	16.862	18.728	64.709	1.00 38.25	В
40	MOTA	1439		ILE	195	17.132	20.092	64.055	1.00 38.19	В
40	ATOM	1440	CG1	ILÈ	195	15.615	18.049	64.084	1.00 39.77	В
	MOTA	1441	CD1	ILE	195	14.321	18.863	64.185	1.00 41.59	В
	MOTA	1442	Ċ	ILE	195	19.347	18.581	65.001	1:00 32.57	В
	ATOM	1443	ō	ILE	195	19.452	18.970	66.162	1.00 30.74	В
	ATOM	1444	N	ILE	196	20.292				
45							18.787	64.086	1.00 29.82	В
47	MOTA	1445	CA	ILE	196	21.500	19.539	64.405	1.00 27.94	В
	MOTA	1446	CB	ILE	196	22.800	18.919	63.769	1.00 26.64	В
	MOTA	1447	CG2	ILE	196	24.006	19.816	64.070	1.00 21.22	В
	MOTA	1448	CG1	ILE	196	23.110	17.510	64.383	1.00 24.18	В
	MOTA	1449		ILE	196	22.375	16.374	63.764	1.00 22.10	В
50	MOTA	1450	С	ILE	196	21.303	20.951	63.872	1.00 27.99	В
	ATOM	1451	ŏ	ILE	196	21.375	21.196	62.669	1.00 27.68	В
	ATOM	1452	N	LYS	197					
						21.044	21.876	64.784	1.00 29.44	В
	MOTA	1453	CA	LYS	197	20.813	23.265	64.426	1.00 30.91	В
E E	MOTA	1454	CB	LYS	197	20.205	24.026	65.616	1.00 33.42	В
55	MOTA	1455	CG	LYS	197	19.931	25.486	65.303	1.00 35.76	В
	MOTA	1456	CD	LYS	197	19.670	26.299	66.548	1.00 39.21	В
	ATOM	1457	CE	LYS	197	19.686	27.776		1.00 42.14	В
	MOTA	1458	NZ	LYS	197	20.909	28.121	65.411	1.00 42.07	В
	MOTA	1459	c	LYS	197	22.073	23.984	63.971		
60		1460							1.00 29.67	В
00	MOTA		0	LYS	197	23.080	23.977	64.674	1.00 29.22	В
	MOTA	1461	N	GLY	198	22.005	24.600	62.792	1.00 29.85	В
	MOTA	1462	CA	GLY	198	23.141	25.345	62.275	1.00 30.66	В
	MOTA	1463	С	GLY	198	24.040	24.637	61.282	1.00 30.74	В
	MOTA	1464	o	GLY	198	24.857	25.283	60.618	1.00 30.16	. B
65	ATOM	1465	N	LEU	199	23.903	23.318	61.178	1.00 30.32	B
	ATOM	1466	CA	LEU	199	24.722			1.00 30.32	
							22.538	60.255		В
	MOTA	1467	CB	LEU	199	24.530	21.004	60.530	1.00 30.24	В
	ATOM	1468	CG	LEU	199	25.328	19.967	59.664	1.00 28.88	В
70	ATOM	1469		LEU	199	26.773	20.398	59.527	1.00 30.22	В
70	MOTA	1470	CD2	LEU	199	25.254	18.587	60.308	1.00 28.26	В
	MOTA	1471	C	LEU	199	24.397	22.869	58.792	1.00 31.25	В
	MOTA	1472	ō	LEU	199	23.256	22.699	58.340	1.00 31.36	В
	MOTA	1473	N	GLU	200	25.406	23.345	58.065		
	514	,,		320	200	23.400	20.043	50.005	1.00 30.26	В

	MOTA	1474	CA	GLU	200	25.253	23.712	56.661	1.00 32.06	В
	ATOM	1475	CB	GLU	200	26.446	24.590	56.190	1.00 34.38	В
	MOTA	1476			200					
			CG	GLU		26.604	25.870	56.961	1.00 41.33	В
_	MOTA	1477	CD	GLU	200	25.395	26.773	56.833	1.00 42.76	В
5	MOTA	1478	OE1	GLU	200	25.121	27.535	57.785	1.00 43.19	В
	ATOM	1479	OE2	GLU	200	24.730	26.721	55.776	1.00 43.56	В
	MOTA		С	GLU	200	25.164	22.514	55.722	1.00 31.83	В
	ATOM	1481	ō	GLU	200	25.841	21.503	55.916		
									1.00 30.83	В
10	MOTA	1482	N	GLU	201	24.328	22.654	54.700	1.00 30.84	В
10	MOTA	1483	CA	GLU	201	24.163	21.639	53.677	1.00 30.37	В
	MOTA	1484	CB	GLU	201	22.732	21.167	53.611	1.00 30.91	В
	MOTA	1485	CG	GLU	201	22.386	20.111	54.629	1.00 33.83	В
	ATOM	1486	CD	GLU	201	20.975	19.587	54.454	1.00 36.02	В
•	ATOM	1487	OE1	GLU	201	20.052			1.00 37.16	
15							20.163	55,069		В
13	MOTA	1488		GLU	201	20.791	18.604	53.695	1.00 36.56	В
	MOTA	1489	C	GLU	201	24.528	22.328	52.373	1.00 30.44	В
	MOTA	1490	0	GLU	201	23.796	23.207	51.919	1.00 30.69	В
	ATOM	1491	N	ILE	202	25.663	21.958	51.783	1.00 28.80	В
	MOTA	1492	CA	ILE	202	26.073	22.575	50.526	1.00 28.82	В
20	ATOM	1493	CB	ILE	202	27.619	22.739	50.409	1.00 28.91	. В
	MOTA	1494		ILE	202	27.978	23.225	49.014	1.00 26.00	В
	MOTA	1495		ILE	202	28.137	23.751	51.426	1.00 28.90	В.
	MOTA	1496	CD1	ILE	202	28.057	23.294	52.863	1.00 32.03	В
	ATOM	1497	С	ILE	202	25.594	21.773	49.324	1.00 28.57	·B
25	MOTA	1498	0	ILE	202	25.844	20.571	49.215	1.00 29.93	В
	ATOM	1499	N	THR	203	24.896	22.448	48.422	1.00 28.23	В
		1500	CA							
	MOTA			THR	203	24.404	21.803	47.219	1.00 26.49	В
	MOTA	1501	CB	THR	203	23:307	22.665	46.527	1.00 26.14	В
20	MOTA	1502	OG1	THR	203	22.173	22.791	47.401	1.00 24.25	В
30	MOTA	1503	CG2	THR	203	22.862	22.028	45.208	1.00 25.01	В
	MOTA	1504	С	THR	203	25.606	21.636	46.293	1.00 26.13	В
	MOTA	1505	ō	THR	203	26.483	22.495	46.253	1.00 26.91	В
	MOTA	1506	N	VAL	204	25.666	20.504	45.599	1.00 26.49	
										В
35 ·	MOTA	1507	CA	VAL	204	26.741	20.220	44.654	1.00 27.51	В
22	MOTA	1508	СB	VAL	204	27.444	18.868	44.967	1.00 25.76	В
	ATOM	1509	CG1	VAL	204	28.653	18.672	44.056	1.00 23.12	В
	MOTA	1510	CG2	VAL	204	27.879	18.837	46.423	1.00 24.79	В
	MOTA	1511	С	VAL	204		20.149	43.321	1.00 29.14	В
	MOTA	1512	ŏ	VAL	204	25.265	19.199	43.061	1.00 30.39	В
40	ATOM	1513	N	HIS	205	26.218	21.170			
70								42.495	1.00 29.22	В
	MOTA	1514	CA	HIS	205	25.553	21.313	41.195	1.00 30.55	В
	MOTA	1515	CB	HIS	205	25.613	22.794	40.767	1.00 28.34	В
	MOTA	1516	CG	HIS	205	25.157	23.732	41.838	1.00 28.46	В
	ATOM	1517	CD2	HIS	205	25.858	24.492	42.711	1.00 27.43	В
45	ATOM	1518	ND1	HIS	205	23.832	23.862	42.196	1.00 28.83	В
	ATOM	1519		HIS	205	23.736	24.654	43.249	1.00 28.44	В
	ATOM	1520		HIS	205	24.952	25.049	43.582	1.00 29.92	В
		1521								
	MOTA		C	HIS	205	26.092	20.435	40.081	1.00 31.51	В
50	MOTA	1522	0	HIS	205	25.358	20.055	39.169	1.00 31.34	В
50	MOTA	1523	N	ASN	206	27.383	20.136	40.147	1.00 33.49	В
	MOTA	1524	CA	ASN	206	28.032	19.299	39.151	1.00 34.62	В
	ATOM	1525	СВ	ASN	206	28.444	20.138	37.930	1.00 34.75	. В
	MOTA	1526	CG	ASN	206	29.164	21.417	38.309	1.00 35.27	В
	MOTA	1527		ASN	206	30.224	21.391	38.938	1.00 37.58	В
55										
"	ATOM	1528	ND2	ASN	206	28.589	22.548	37.925	1.00 34.11	В
	ATOM	1529	С	ASN	206	29.243	18.650	39.798	1.00 35.69	В
	MOTA	1530	0	ASN	206	29.478	18.836	40.992	1.00 36.45	В
	MOTA	1531	N	LYS	207	30.002	17.876	39.031	1.00 36.43	₿.
	MOTA	1532	CA	LYS	207	31.171	17.216	39.590	1.00 38.62	В
60	MOTA	1533	СВ	LYS	207	31.582	15.993	38.703	1.00 40.10	В
	ATOM	1534	CC	LYS	207					
						32.123	16.339	37.319	1.00 42.56	В
	MOTA	1535	CD	LYS	207	32.259	15.081	36.456	1.00 44.26	В
	MOTA	1536	CE	LYS	207	33.191	15.293	.35.267	1.00 43.78	В
	MOTA	1537	NZ	LYS	207	34.613	15.454	35.696	1.00 42.46	В
65	ATOM	1538	С	LYS	207	32.313	18.222	39.700	1.00 39.03	В
	ATOM	1539	ŏ	LYS	207	33.176	18.120	40.576	1.00 38.73	В
	ATOM	1540	N	ASP	208	32.292	19.208			
								38.813	1.00 39.88	В
	MOTA	1541	CA	ASP	208	33.312	20.244	38.790	1.00 40.76	В
70	ATOM	1542	CB	ASP	208	33.248	20.981	37.461	1.00 42.58	В
70	ATOM	1543	CG	ASP	208	33.659	20.101	36.292	1.00 45.91	В
	ATOM	1544	OD1	ASP	208	33.407	20.484	35.127	1.00 46.74	В
	ATOM	1545		ASP	208	34.246	19.023	36.542	1.00 46.78	В
	ATOM	1546	C	ASP	208	33.141	21.219	39.952	1.00 39.55	В
			-	,						

	MOTA	1547	0	ASP	208	33.643	22.339	39.922	1.00 41.22	В
	MOTA	1548	Ŋ	GLU	209	32.457	20.784	40.996	1.00 37.46	В
	MOTA	1549	ÇA	GLU	209	32.241	21.660	42.128	1.00 35.89	В
_	MOTA	1550	CB	GLU	209	30.760	22.075	42.158	1.00 35.84	В
5	MOTA	1551	CG	GLU	209	30.445	23.275	43.010	1.00 37.17	В
	MOTA	1552	CD	GLU	209	28.973	23.682	42.924	1.00 38.94	В
	MOTA	1553		GLU	209	28.462	23.857	41.793	1.00 37.72	В
	MOTA	1554	OE2	GLU	209	28.327	23.835	43.988	1.00 38.77	В
	ATOM	1555	c	GLU	209	32.646		43.439	1.00 34.61	B
10	MOTA	1556	ŏ	GLU	209	32.763	21.657	44.470	1.00 36.51	В
	MOTA	1557	N	VAL	210	32.907	19.690	43.395	1.00 32.07	B
	MOTA	1558	CA	VAL	210	33.268	18.966	44.609	1.00 32.07	В
	ATOM	1559	CB	VAL	210	33.065	17.411	44.450	1.00 29.01	В
	ATOM	1560			210	31.856			1.00 26.09	
15							17.110	43.574		В
13	ATOM	1561	CG2		210	34.301	16.774	43.901	1.00 29.03	В
	MOTA	1562	C	VAL	210	34.668	19.212	45.183	1.00 28.45	. В
	ATOM		. 0	VAL	210	34.820	19.322	46.406	1.00 29.31	В
	MOTA	1564	N	TYR	211	35.694	19.311	44.343	1.00 26.40	В
20	MOTA	1565	CA	TYR	211	37.038	19.505	44.894	1.00 24.93	В
20	MOTA	1566	CB	TYR	211	38.106	19.552	43.783	1.00 22.02	В
	MOTA	1567	CG	TYR	. 211	39.510	19.386	44.318	1.00 23.83	В
	ATOM	1568		TYR	211	39.850	18.284	45.097	1.00 26.06	В
	MOTA	1569	CE1		211	41.136	18.131	45.625	1.00 25.76	В
25	MOTA	1570		TYR	211	40.498	20.339	44.074	1.00 24.90	В
25	MOTA	1571	CE2		211	41.790	20.196	44.597	1.00 24.81	В
	ATOM	1572	cz	TYR	211	42.103	19.089	45.374	1.00 25.75	. В
	MOTA	1573	ОН	·TYR	211	43.373	18.938	45.910	1.00 23.97	В
	MOTA	1574	С	TYR	211	37.111	20.759	45.757	1.00 25.45	В
~~	MOTA	1575	0	TYR	211	37.691	20.740	46.844	1.00 24.21	В
30	MOTA	1576	N	GLN	212	36.501	21.840	45.272	1.00 27.99	В
	MOTA	1577	CA	GLN	212	36.473	23.117	45.983	1.00 27.45	В
	MOTA	1578	CB	GLN	212	35.721	24.126	45.163	1.00 31.66	В
	MOTA	1579	CG	GLN	212	35.365	25.402	45.907	1.00 37.63	В
	MOTA	1580	CD	GLN	212	35.696	26.654	45.105	1.00 40.53	В
35	ATOM	1581	OE1	GLN	212	35.305	26.782	43.937	1.00 39.59	в.
	MOTA	1582	NE2	GLN	212	36.418	27.587	45.731	1.00 39.73	В
	MOTA	1583	С	GLN	212	35.834	22.981	47.364	1.00 26.73	В
	ATOM	1584	0	GLN	212	36.329	23.527	48.347	1.00 26.01	В
	ATOM	1585	N	ILE	213	34.733	22.243	47.437	1.00 26.10	В
40	ATOM	1586	CA	ILE	213	34.044	22.037	48.703	1.00 24.91	В
. •	MOTA	1587	СВ	ILE	213	32.694	21.327	48.496	1.00 23.51	В
	MOTA	1588		ILE	213	31.978	21.200	49.835	1.00 20.39	В
	ATOM	1589		ILE	213	31.843	22.117	47.461	1.00 22.89	В
	MOTA	1590	CD1		213	30.472	21.509	47.152	1.00 23.13	В
45	ATOM	1591	C	ILE	213	34.906	21.207	49.656	1.00 25.49	В
	ATOM	1592	ŏ	ILE	213	34.916	21.448	50.865	1.00 24.30	В
	ATOM	1593	N	LEU	214	35.618	20.226	49.106	1.00 26.92	В
	ATOM	1594	CA	LEU	214	36.496	19.381	49.905	1.00 28.92	
	MOTA	1595	CB	LEU	214					В
50	ATOM	1596	CG	LEU	214	37.031	18.168	49.050 49.152	1.00 28.21 1.00 30.13	В
50						36.272	16.802			В
	ATOM	1597 1598		LEU	214	34.796	17.034	49.411	1.00 31.20	В
	MOTA				214	36.482	15.987	47.876	1.00 29.12	В
	MOTA	1599	C	LEU	214	37.657	20.225	50.442	1.00 29.28	В
55	ATOM	1600	0	LEU	214	38.012	20.114	51.620	1.00 30.45	В
55	MOTA	1601	N	GLU	215	38.235	21.083	49.599	1.00 28.08	В
	ATOM	1602	CA	GLU	215	39.339	21.932	50.059	1.00 28.89	В
	MOTA	1603	СВ	GLU	215	39.864	22.842	48.914	1.00 29.69	В
	MOTA	1604	CG	GLU	215	40.426	22.093	47.714	1.00 33.51	В
60	ATOM	1605	CD	GLU	215	41.092	23.014	46.700	1.00 36.27	В
UU	MOTA	1606		GLU	215	42.343	23.136	46.730	1.00 34.34	В
	ATOM	1607		GLU	215	40.358	23.620	45.880	1.00 36.57	В
	MOTA	1608	C	GLU	215	38.919	22.795	51.255	1.00 28.03	В
	MOTA	1609	0	GLU	215	39.682	22.953	52.210	1.00 27.31	B _.
45	MOTA	1610	N	LYS	216	37.707	23.348	51.204	1.00 27.99	В
65	MOTA	1611	CA	LYS	216	37.202	24.183	52.290	1.00 29.52	В
	MOTA	1612	CB	LYS	216	35.799	24.696	51.971	1.00 30.11	В
	MOTA	1613	CG	LYS	216	35.691	25.416	50.650	1.00 32.53	В
	MOTA .	1614	CD	LYS	216	36.584	26.643	50.602	1.00 34.31	В
	MOTA	1615	CE	LYS	216	36.596	27.272	49.200	1.00 36.64	В
70	MOTA	1616	NZ	LYS	216	37.248	26.419	48.152	1.00 34.44	В
	MOTA	1617	С	LYS	216	37.170	23:415	53.609	1.00 30.05	В
	MOTA	1618	0	LYS	216	37.516	23.960	54.658	1.00 31.96	В
	MOTA	1619	N	GLY	217	36.742	22.156	53.553	1.00 30.83	В

•	MOTA	1620	CA	GLY	217	36.695	21.335	54.752	1.00 29.82	В
	MOTA	1621	С	GLY	217	38.107	21.144	55.270	1.00 29.77	В
	ATOM	1622	0	GLY	217	38.389	21.354	56.460	1.00 28.73	В
	MOTA	1623	N	ALA	218	39.000	20.749	54.363	1.00 29.20	В
5	MOTA	1624	ĊA	ALA	218	40.404	20.548	54.696	1.00 28.09	В
	MOTA	1625	СВ	ALA	218	41.212	20.299	53.427	1.00 25.39	В
	MOTA	1626	Č	ALA	218	40.924	21.792	55.422	1.00 27.61	В
	ATOM	1627	ŏ	ALA	218	41.623	21.684	56.429	1.00 27.17	В
	MOTA	1628	N	ALA	219	40.559	22.969	54.914	1.00 27.54	В
10	ATOM	1629	CA	ALA	219	40.984	24.243			
10								55.505	1.00 27.45	В
	MOTA	1630 1631	CB	ALA	219	40.430	25.406	54.695	1.00 26.20	В
	MOTA		Ç	ALA	219	40.553	24.385	56.964	1.00 27.16	В
•	MOTA	1632	0	ALA	219	41.368	24.726	57.833	1.00 26.05	В
15	MOTA	1633	N	LYS	220	39.273	24.135	57.227	1.00 26.17	В
13	MOTA	1634	CA	LYS	220	38.754	24.234	58.585	1.00 26.59	В
	MOTA	1635	CB	LYS	220	37.203	24.057	58.592	1.00 25.82	В
	MOTA	1636	CG	LYS	220	36.477	25.037	57.691	1.00 26.36	В
	MOTA	1637	CD	LYS	220	34.997	25.195	58.065	1.00 28.61	В
20	MOTA	1638	CE	LYS	220	34.827	25.771	59.471	1.00 27.13	В
20	ATOM	1639	NZ	LYS	220	33.406	26.129	59.789	1.00 25.98	В
	MOTA	1640	C	LYS	220	39.426	23.190	59.491	1.00 26.00	В
	MOTA	1641	0	LYS	220	39.715	23.465	60.665	1.00 24.88	В.
	ATOM	1642	N	ARG	221	39.671	22.000	58.937	1.00 24.80	В
25	ATOM	1643	CA	ARG	221	40.330	20.916	59.671	1.00 22.73	·B
25	ATOM	1644	CB	ARG	221	40.685	19.757	58.725	1.00 24.70	В
	ATOM	1645	CG	ARG	221	39.524	18.885	58.293	1.00 25.62	В
	ATOM	1646	CD	ARG	221	39.367	17.736	59.256	1.00 26.10	В
	MOTA	1647	NE	ARG	221	. 38:190	16.934	58.960	1.00 24.76	В
20	ATOM	1648	CZ	ARG	221	38.065	16.146	57.901	1.00 22.87	. В
30	MOTA	1649	NH1	ARG	221	39.061	16.051	57.021	1.00 19.50	В
	MOTA	1650	NH2	ARG	221 [.]	36.942	15.451	57.735	1.00 20.09	В
	MOTA	1651	С	ARG	221	41.624	21.456	60.267	1.00 21.95	· в
	MOTA	1652	0	ARG	221	41.889	21.306	61.466	1.00 20.88	В
25.	MOTA	1653	N	THR	222	42.421	22.089	59.406	1.00 20.21	В
35 ·	ATOM	1654	CA	THR	222	43.705	22.661	59.795	1.00 19.39	В
	ATOM	1655	CB	THR	222	44.312	23.464	58.650	1.00 21.09	В
	MOTA	1656	OG1	THR	222	44.502	22.600	57.525	1.00 22.38	В
	ATOM	1657	CG2	THR	222	45.649	. 24.077	59.073	1.00 20.44	В
40	ATOM	1658	С	THR	222	43.589	23.579	60.991	1.00 18.28	В
40	ATOM	1659	0	THR	222	44.338	23.441	61.952	1.00 17.80	В
	ATOM	1660	N	THR	223	42.649	24.517	60.926	1.00 17.37	В
	MOTA	1661	CA	THR	223	42.452	25.461	62.012	1.00 18.66	В
	MOTA	1662	CB	THR	223	41.496	26.590	61.605	1.00 17.71	В
	MOTA	1663	0G1	THR	223	40.245	26.413	62.268	1.00 20.08	В
45	ATOM	1664	CG2	THR	223	41.258	26.581	60.111	1.00 16.54	В
	ATOM	1665	С	THR	223	41.902	24.740	63.242	1.00 20.76	В
	MOTA	1666	Q .	THR	223	42.206	25.120	64.374	1.00 24.08	В
	ATOM	1667	N	ALA	224	41.100	23.698	63.018	1.00 21.47	В
	ATOM	1668	CA	ALA	224	40.529	22.898	64.105	1.00 19.87	В
50	ATOM	1669	CB	ALA	224	39.642	21.801	63.534	1.00 22.14	В
	MOTA	1670	С	ALA	224	41.667	22.266	64.894	1.00 19.87	В
	MOTA	1671	0	ALA	224	41.689	22.289	66.129	1.00 16.71	В
	ATOM	1672	N	ALA	225	42.604	21.680	64.155	1.00 20.37	В
	ATOM	1673	CA	ALA	225	43.765	21.048	64.755	1.00 20.88	В
55	ATOM	1674	CB	ALA	225	44.647	20.440	63.666	1.00 19.50	В
	ATOM	1675	С	ALA	225	44.541	22.096	65.553	1.00 22.18	В
	ATOM	1676	0	ALA	225	45.054	21.808	66.638	1.00 20.94	B
	ATOM	1677	N	THR	226	44.613	23.319	65.023	1.00 23.92	В.
	MOTA	1678	CA	THR	226	45.324	24.401	65.717	1.00 24.83	В
60 ·	ATOM	1679	CB	THR	226	45.313	25.723	64.895	1.00 24.59	В
	MOTA	1680		THR	226	46.088	25.565	63.699	1.00 23.18	В,
	ATOM	1681		THR	226	45.904	26.866	65.721	1.00 25.23	B
	MOTA	1682	c	THR	226	44.699	24.679	67.089	1.00 25.25	В
	MOTA	1683	ō	THR	226	45.405	24.877	68.083	1.00 25.41	В
65	MOTA	1684	N	LEU	227		24.680	67.130	1.00 25.12	В
	MOTA	1685	CA	LEU	227	42.619	24.000	68.353	1.00 25.47	
	MOTA	1686	CB	LEU	227	41.222	25.541	67.980	1.00 28.90	В
	ATOM	1687	CG	LEU	227	41.222	27.041	67.561		В
	ATOM	1688		LEU	227				1.00 32.68	В
70	MOTA	1689		LEU	227	42.240 39.756	27.567	66.763	1.00 31.51	В
, 0	ATOM	1690	CDZ	LEU	227		27.156 23.739	66.755	1.00 32.75	В
	ATOM	1691	0	LEU	227	42.409 42.348		69.296		В
	MOTA	1692	N	MET	227		23.906	70.520	1.00 25.50	В
	A I OPI	1032	74	ric I	220	42.295	22.533	68.755	1.00 24.99	В

	MOTA	1693	ÇA	MET	228	42.041	21.392	69.635	1.00 25.58	В
	MOTA	1694	CB	MET	228	40.625	20.786	69.310	1.00 27.00	В
	MOTA	1695	CG	MET	228	39.499	21.798	69.554	1.00 28.30	В
	MOTA	1696	SD	MET	228	37.874	21.368	68.919	1.00 31.74	
5										В
,	MOTA	1697	CE	MET	228	37.998	22.026	67.265	1.00 30.21	В
	MOTA	1698	C .	MET	228	43.091	20.301	69.666	1.00 23.55	В
	MOTA	1699	0	MET	228	43.547	19.828	68.629	1.00 23.83	В
	MOTA	1700	N	ASN	229	43.471	19.913	70.882	1.00 22.85	В
	ATOM	1701	CA	ASN	229	44.470	18.870	71.099	1.00 21.02	В
10	ATOM	1702	CB	ASN	229	44.574	18.524	72.588	1.00 19.32	В
~~	ATOM	1703	CG	ASN	229					
						45.172	19.646	73.426	1.00 19.33	В
	MOTA	1704	OD1		229	45.690	20.634	72.899	1.00 19.44	В
	MOTA	1705		ASN	229	45.112	19.484	74.751	1.00 13.92	В
	MOTA	1706	C	ASN	229	44.162	17.582	70.329	1.00 21.09	В
15	MOTA	1707	0	ASN	229	43.063	17.026	70.435	1.00 21.09	В
	MOTA	1708	N	ALA	230	45.144	17.121	69.558	1.00 20.25	В
	ATOM	1709	CA	ALA	230	45.030	15.887	68.786	1.00 19.42	B
	ATOM	1710	CB	ALA	230	45.224	14.675		1.00 21.67	
								69.721		В
20	MOTA	1711	C	ALA	230	43.694	15.783	68.067	1.00 18.26	В
20	MOTA	1712	0	ALA	230	43.096	14.712	68.000	1.00 17.83	В
	MOTA	1713	N	TYR	231	43.242	16.897	67.512	1.00 17.17	В
	ATOM ·	1714	CA	TYR	231	41.965	16.927	66.821	1.00 17.72	В
	MOTA	1715	CB	TYR	231	41.694	18.379	66.201	1.00 15.95	В
	ATOM	1716	CG	TYR	231	40.341	18.465	65.524	1.00 12.55	B
25	ATOM	1717	CD1	TYR	231	40.205	18.269	64.151		
45									1.00 12.28	·B
	MOTA	1718	CE1		231	38.933	18.219	63.555		. В
	MOTA	1719		TYR	231	39.182	18.621	66.279	1.00 10.61	В
	MOTA	1720	CE2	TYR	231	37.918	18.573	65.690	1.00 9.26	В
	ATOM	1721	CZ	TYR	231	37.802	18.372	64.338	1.00 6.19	В
30	ATOM	1722	ОН	TYR	231	36.545	18.335	63.777	1.00 8.98	В
	ATOM	1723	C	TYR	231	41.728	15.869	65.731	1.00 18.14	В
	ATOM	1724	ŏ	TYR	231	40.596		65.571	1.00 17.92	
							15.392			В
	MOTA	1725	N	SER	232	42.769	15.504	64.982	1.00 17.34	В
25	MOTA	1726	CA	SER	232	42.585	14.537	63.903	1.00 17.96	В
35	MOTA	1727	CB	SER	232	43.681	14.688	62.816	1.00 13.72	В
	MOTA	1728	0G	SER	232	44.941	14.251	63.275	1.00 15.73	В
	MOTA	1729	С	SER	232	42.502	13.070	64.323	1.00 18.78	В
	ATOM	1730	ŏ	SER	232	41.934	12.255	63.598	1.00 19.24	В
	ATOM	1731	N	SER	233					
40						43.051	12.726	65.480	1.00 17.77	В
70	MOTA	1732	CA	SER	233	43.019	11.340	65.904	1.00 16.56	В
	MOTA	1733	СB	SER	233	44.383	10.932	66.496	1.00 18.00	В
	MOTA	1734	OG	SER	233	44.509	11.362	67.846	1.00 17.89	В
	ATOM	1735	С	SER	233	41.935	11.141	66.943	1.00 17.20	B
	MOTA	1736	0	SER	233	41.413	10.035	67.110	1.00 13.55	В
45	MOTA	1737	N	ARG	234	41.570	12.235	67.609	1.00 18.37	В
	MOTA	1738	CA	ARG	234	40.579	12.185	68.678		
									1.00 18.14	В
	MOTA	1739	СВ	ARG	234	41.035	13.079	69.848	1.00 20.04	В
	MOTA	1740	CG	ARG	234	41.136	12.352	71.169	1.00 23.36	В
	MOTA	1741	CD	ARG	234	42.547	12.392	71.767	1.00 25.39	В
50	MOTA	1742	NE	ARG	234	42.847	13.651	72.455	1.00 28.46	В
	MOTA	1743	CZ	ARG	234	43.898	13.844	73.255	1.00 28.83	В
	MOTA	1744	NH1	ARG	234	44.765	12.865	73.479	1.00 28.24	В
	MOTA	1745	NH2		234	44.082	15.019	73.842	1.00 28.56	В
	ATOM	1746	C	ARG		39.142				
55					234		12.524	68.318	1.00 17.12	В
"	MOTA	1747	0	ARG	234	38.262	12.440	69.174	1.00 16.45	В
	MOTA	1748	N	SER	· 235	38.879	12.876	67.064	1.00 17.25	В
	MOTA	1749	CA	SER	235	37.508	13.232	66.685	1.00 17.01	В
	MOTA	1750	CB	SER	235	37.470	14.581	66.108	1.00 16.15	В
	MOTA	1751	OG	SER	235	38.109	14.594	64.847	1.00 15.24	В
60	ATOM	1752	Č	SER	235	36.847	12.297	65.697	1.00 17.23	
••	ATOM									В
		1753	0	SER	235	37.505	11.536	64.991	1.00 17.87	В
	MOTA	1754	N	HIS	236	35.527	12.381	65.655	1.00 16.90	В
	MOTA	1755	CA	HIS	236	34.720	11.580	64.750	1.00 18.47	В
	ATOM	1756	CB	HIS	236	33.553	10.961	65.484	1.00 20.05	B
65	MOTA	1757	CG	HIS	236	33.941	10.192	66.705	1.00 21.39	В
	MOTA	1758		HIS	236	33.907	10.529	68.016	1.00 20.87	В
	ATOM	1759		HIS	236	34.444	8.910	66.650	1.00 20.87	В
	ATOM	1760		HIS						
					236	34.700	8.490	67.876	1.00 20.80	В
70	MOTA	1761		HIS	236	34.385	9.454	68.723	1.00 19.15	В
70	MOTA	1762	Ç	HIS	236	34.166	12.518	63.688	1.00 19.93	В
	MOTA	1763	0	HIS	236	33.598	13.569	64.005	1.00 18.38	В
	ATOM	1764	N	SER	237	34.326	12.155	62.425	1.00 20.64	В
	MOTA	1765	CA	SER	237	33.795	13.001	61.374	1.00 21.44	В
					•					_

	•									
•	MOTA	1766	CB	SER	237	34.889	13.424	60.424	1.00 20.37	В
	MOTA	1767	OG	SER	237	35.258	12.370	59.566	1.00 19.17	В
	MOTA	1768	С	SER	237	32.731	12.224	60.619	1.00 21.91	В
	ATOM	1769	ō	SER	237	32.908	11.043	60.320	1.00 21.18	В
5	ATOM	1770	N	VAL	238	31.620	12.886	60.324	1.00 21.76	В
	MOTA	1771	CA	VAL	238	30.548	12.246	59.587	1.00 22.83	В
	MOTA		CB	VAL	238	29.297	12.024	60.475	1.00 25.08	В
•	ATOM	1773	CG1	VAL	238	29.043	13.241	61.323	1.00 27.25	В
	ATOM	1774	CG2	VAL	238	28.077	11.717	59.601	1.00 24.91	В
10	ATOM	1775	С	VAL	238	30.176	13.052	58.366	1.00 21.64	В
	MOTA	1776	·ō	VAL	238	29.399	13.986	58.450	1.00 24.16	В
	MOTA	1777	N	PHÉ	239	30.764	12.683	57.232	1.00 23.48	B
	ATOM	1778	CA	PHE	239	30.513	13.331	55.943	1.00 23.45	В
1 =	MOTA	1779	CB	PHE	239	31.736	13,139	55.002	1.00 22.63	В
15	MOTA	1780	CG	PHE	239	31.658	13.923	53.722	1.00 20.75	В
	ATOM	1781	CD1	PHE	239	30.660	13.667	52.785	1.00 19.42	В
•	ATOM	1782		PHE	239	32.580	14.928	53.458	1.00 20.63	B
	ATOM	1783		PHE	239	30.578	14.403	51.596		
									1.00 21.05	В
20	MOTA	1784		PHE	239	32.510	15.676	52.268	1.00 21.14	В
20	ATOM	1785	CZ	PHE	239	31.506	15.413	51.334	1.00 19.84	В
	ATOM	1786	С	PHE	239	29.286	12.669	55.321	1.00 24.62	В
	MOTA	1787	0	PHE	239	29.326	11.482	54.983	1.00 24.57	В.
	ATOM	1788	N	SER	240	28.202	13.430	55.178	1.00 24.38	В
	MOTA	1789	CA	SER	240	26.968	12.910	54.596	1.00 23.26	· B
25	MOTA	1790	СВ	SER	240	25.778	13.249	55.480	1.00 22.32	
	ATOM									В
		1791	OG	SER	240	25.932	12.724	56.786	1.00 21.48	В
	MOTA	1792	C	SER	240	26.704	13.447	53.199	1.00 23.92	В
	MOTA	1793	0	SER	240	27.065	14.568	52.865	1.00 23.73	В
	MOTA	1794	N	VAL	241	26.067	12.622	52.382	1.00 25.40	· в
30	MOTA	1795	CA	VAL	241	25.712	12.995	51.022	1.00 25.45	В
	MOTA	1796	СВ	VAL	241	26.654	12.349	49.985	1.00 26.85	В
	ATOM	1797		VAL	241	26.790	10.856	50.249	1.00 26.88	B
	ATOM	1798		VAL	241		12.595			
						26.118		48.579	1.00 26.95	. В
35	MOTA	1799	C	VAL	241	24.293	12.513	50.787	1.00 25.56	B
33	ATOM '	1800	0	VAL	241	24.013	11.321	50.856	1.00 25.33	В
•	ATOM	1801	N .	THR	242	23.391	13.454	50.536	1.00 26.85	В
	MOTA	1802	CA	THR	242	21.996	13.130	50.302	1.00 26.02	В
	MOTA	1803	ÇВ	THR	. 242	21.091	13.997	51.182	1.00 26.36	В
	MOTA	1804		THR	242	21.447	13.814	52.557	1.00 26.94	В
40	MOTA	1805		THR	242	19.628	13.612	50.995	1.00 28.00	B
. •	MOTA	1806		THR	242					
			Č			21.656	13.352	48.832	1.00 27.35	В
	MOTA	1807	Ŏ.	THR	242	22.126	14.311	48.217	1.00 26.21	В
	MOTA	1808	N	ILE	243	20.857	12.451	48.263	1.00 28.40	В
	ATOM	1809	CA	ILE	243	20.468	12.564	46.861	1.00 28.65	В
45	ATOM	1810	CB	ILE	243	21.048	11.407	46.017	1.00 28.29	В
	ATOM	1811	CG2	ILE	243	20.944	11.746	44.534	1.00 27.94	В
	ATOM	1812		ILE	243	22.526	11.156	46.392	1.00 29.06	B
	ATOM	1813			243	23.191	10.046			
								45.592	1.00 25.36	В
50	MOTA	1814	C :	ILE	243	18.950	12.538	46.721	1.00 29.68	В
<i>5</i> 0	ATOM	1815	0	ILE	243	18.327	11.512	46.966	1.00 30.63	В
	ATOM .	1816	N	HIS	244	18.355	13.672	46.358	1.00 31.77	В
	MOTA	1817	CA	HIS	244 .	16.908	13.744	46.158	1.00 32.56	. В
	ATOM	1818	CB	HIS	244	16.354	15.175	46.421	1.00 33.70	В
	ATOM	1819	CG	HIS	244	16.323	15.570	47.864	1.00 34.78	В
55	MOTA	1820		HIS	244	15.331	15.500	48.785	1.00 35.77	В
	ATOM	1821		HIS	244					
						17.405	16.132	48.511	1.00 36.48	В
	ATOM	1822	CE1		244	17.080	16.392	49.765	1.00 35.67	В
	MOTA	1823	NE2		244	15.827	16.018	49.958	1.00 35.06	₿.
	ATOM	1824	С	HIS	244	16.700	13.383	44.693	1.00 33.70	В
60 ·	MOTA	1825	0	HIS	244	17.271	14.020	43.798	1.00 33.29	В
	MOTA	1826	N	MET	245	15.885	12.366	44.448	1.00 34.30	В
	ATOM	1827	CA	MET	245	15.654	11.910	43.087	1.00 34.70	
	MOTA	1828	CB	MET	245		10.483			В
						16.212		.42.944	1.00 34.85	В
65	MOTA	1829	CG	MET	245	17.734	10.441	43.100	1.00 35.80	В
UJ	ATOM	1830	SD	MET	245	18.439	8.805	43.321	1.00 36.13	В
	MOTA	1831	CE	MET	245	18.009	8.537	45.032	1.00 32.87	В
	MOTA	1832	С	MET	245	14.203	11.985	42.628	1.00 34.49	В
	MOTA	1833	0	MET	245	13.272	11.757	43.402	1.00 33.49	. В
	MOTA	1834	N	LYS	246	14.026	12.313	41.352	1.00 35.05	. В
70	ATOM	1835	CA	LYS	246					
. •						12.700	12.449	40.769	1.00 36.99	В
	ATOM	1836	CB	LYS	246	12.280	13.947	40.750	1.00 38.69	В
	ATOM	1837	CG.	LYS	246	10.919	14.227	40.117	1.00 43.46	В
	MOTA	1838	CD	LYS	246	10.702	15.729	39.856	1.00 45.60	В

	ATOM	1839	CE	LYS	246	10.795	16.556	41.148	1.00 48.45	. В
	MOTA	1840	NZ	LYS	246	10.619	18.031	40.940	1.00 46.59	В
	ATOM	1841		LYS	246	12.654	11.889	39.353	1.00 36.70	В
			C							
5	MOTA	1842	0	LYS	246	13.324	12.387	38.452	1.00 36.63	В
)	MOTA	1843	N	GLU	247	11.864	10.841	39.166	1.00 36.80	В
	ATOM .	1844	CA	GLU	247	11.706	10.240	37.854	1.00 37.12	В
	ATOM	1845	CB	GLU	247	12.209	8.806	37.866	1.00 37.24	В
	ATOM	1846	CG	GLU	247	11.710	7.990	39.036	1.00 37.73	В
	MOTA	1847	CD	GLU	247	12.621		39.347	1.00 38.20	В
10	MOTA	1848		GLU	247	12.293	6.035	40.262	1.00 37.07	В
	ATOM	1849		GLU	247	13.670	6.692	38.677	1.00 38.76	В
						•				
	MOTA	1850	C	GLU	247	10.228	10.299	37.498	1.00 36.40	В
	MOTA	1851	0	GLU	247	9.369	10.193	38.365	1.00 35.41	В
1 5	MOTA	1852	N	THR	248	9.940	10.498	36.219	1.00 37.67	В
15	MOTA	1853	CA	THR	248	8.563	10.587	35.746	1.00 39.02	В
	MOTA	1854	ÇВ	THR	248	8.344	11.889	34.920	1.00 39.40	В
	MOTA	1855	. OG1	THR	248	8.754	13.025	35.693	1.00 40.65	В
	ATOM	1856	CG2	THR	248	6.877	12.050	34.543	1.00 40.08	В
	MOTA	1857	C	THR	248	8.240	9.381	34.863	1.00 39.45	В
20	ATOM	1858	ō	THR	248	8.959	9.095	33.902	1.00 39.20	В
	ATOM	1859	N	THR	249	7.158	8.678	35.187	1.00 39.85	В
	ATOM .	1860	CA	THR	249	6.751	7.515	34.407		В
	ATOM	1861	CB	THR	249	5.642	6.728	35.119	1.00 41.31	В
25	ATOM	1862	0G1		249	4 458	7.531	35.190	1.00 40.33	В
25	MOTA	1863	CG2	THR	249	6.078	6.345	36.527	1.00 39.92	В
	MOTA	1864	С	THR	249	6.233	7.952	33.039	1.00 41.94	. В
	MOTA	1865	0	THR	249	6.178	9.145	32.736	1.00 41.92	В
	MOTA	1866	N	ILE	250	5.857	6.979	32.214	1.00 43.64	В
	MOTA	1867	CA	ILE	250	5.343	7.253	30.875	1.00 43.57	В
30	MOTA	1868	CB	ILE	250	5.340	5.970	30.004	1.00 43.38	В
-	MOTA	1869		ILE	250	4.228	5.029	30.465	1.00 41.86	
										В
	MOTA	1870		ILE	250	5.173	6.343	28.510	1.00 41.89	В
	MOTA	1871		ILE	250 .	5.286	5.169	27.560	1.00 39.31	В
25	MOTA	1872	C	ILE	250	3.922	7.805	30.983	1.00 44.06	В
35	MOTA	1873	0	ILE	250	3.320	8.197	29.984	1.00 43.16	В.
	MOTA	1874	N	ASP	251	3.402	7.834	32.209	1.00 45.37	В
	ATOM	1875	CA	ASP	251	2.059	8.353	32.493	1.00 47.36	В
	ATOM	1876	СВ	ASP	251	1.319	7.437	33.502	1.00 47.52	В
	MOTA	1877	CG	ASP	251	0.719	6.208	32.852	1.00 46.95	В
40	MOTA	1878		ASP	251	0.222	5.335	33.595	1.00 46.42	B
+0										
	MOTA	1879		ASP	251	0.735	6.121	31.606	1.00 46.77	В
	MOTA	1880	C	ASP	251	2.097	9.778	33.061	1.00 48.00	В
	MOTA	1881	0	ASP	251	1.052	10.349	33.377	1.00 49.62	В
4.5	ATOM	1882	N	GLY	252	3.297	10.339	33.195	1.00 48.57	В
45	MOTA	1883	CA	GLY	252	3.445	11.684	33.725	1.00 48.41	В
	MOTA	1884	С	GLY	252	3.519	11.749	35.243	1.00 49.25	В
	MOTA	1885	0	GLY	252	3.592	12.839	35.823	1.00 48.30	В
	MOTA	1886	N	GLU	253	3.489	10.584	35.890	1.00 49.52	В
	ATOM	1887	CA	GLU	253	3.555	10.504	37.349	1.00 49.94	В
50	MOTA	1888	CB	GLU	253	2.989	9.156	37.839	1.00 51.87	В
••	MOTA	1889	CG	GLU	253	3.083	8.942	39.349	1.00 55.20	В
	ATOM	1890	CD	GLU	253	2.805	7.498	39.764	1.00 57.60	
										В
	MOTA	1891		GLU	253	2.837	7.204	40.981	1.00 58.27	В
55	ATOM	1892		GLU	253	2.558	6.655	38.875	1.00 58.42	В
22	MOTA	1893	С	GLU	253	4.996	10.659	37.835	1.00 49.08	В
	ATOM	1894	0	GLU	253	5.948	10.301	37.136	1.00 47.88	В
	MOTA	1895	N	GLU	254	5.148	11.187	39.043	1.00 48.18	В
	MOTA	1896	CA	GLU	254	6.471	11.394	39.610	1.00 48.03	В
	MOTA	1897	CB	GLU	254	6.633	12.854	40.000	1.00 48.74	В
60	ATOM	1898	CG	GLU	254	6.950	13.761	38.827	1.00 51.39	В
	ATOM	1899	CD	GLU	254	6.866	15.232	39.193	1.00 53.81	В
	ATOM	1900		GLU	254					
	ATOM	1901		GLU	254	7.184 6.493	15.575 16.043	40.356 38.313	1.00 54.50	В
									1.00 54.20	В
65	MOTA	1902	C	GLU	254	6.817	10.497	40.797	1.00 46.73	B `
U.J	MOTA	1903	0	GLU	254	6.111	10.466	41.805	1.00 46.07	В
	MOTA	1904	N	LEU	255	7.918	9.763	40.651	1.00 45.44	В
	MOTA	1905	CA	LEU	255	8.416	8.869	41.689	1.00 43.34	В
	ATOM .	1906	CB	LEU	255	8.880	7.522	41.069	1.00 42.70	В
	MOTA	1907	CG	LEU	255	7.888	6.755	40.138	1.00 42.10	В
70	MOTA	1908		LEU	255	8.584	5.548	39.528	1.00 41.93	В
-	MOTA	1909		LEU	255	6.658	6.322	40.919	1.00 42.42	В
	MOTA	1910	C	LEU	255	9.603	9.591	42.329	1.00 42.42	
	ATOM									В
	AIOM	1911	0	LEU	255	10.599	9.886	41.662	1.00 40.70	В

	ATOM	1912	N	VAL	256		9.484	9.890	43.617	1.00 41.65	В
	ATOM	1913	CA	VAL	256		10.540	10.594	44.326	1.00 41.53	В
	ATOM	1914	CB	VAL	256		9.994	11.865	45.040	1.00 42.73	В
	ATOM	1915		VAL	256		9.445	12.851	44.013	1.00 41.79	В
5	ATOM	1916		VAL	256		8.899	11.487	46.028	1.00 43.14	В
-	MOTA	1917		VAL	256			9.691			
			C				11.192		45.357	1.00 40.91	В
	ATOM '	1918	0	VAL	256			9.123	46.216	1.00 42.52	В
	MOTA	1919	N	LYS	257		12.507	9:542	45.255	1.00 38.10	В
10	MOTA	1920	CA	LYS	257		13.237	8.718	46.200	1.00 35.97	В
10	MOTA	1921	CB	LYS	257		13.712	7.370	45.525	1.00 37.07	В
	MOTA	1922	CG	LYS	257		14.482	7.490	44.219	1.00 35.97	В
	MOTA	1923	CD	LYS	257		14.612	6.108	43.592	1.00 34.96	В
	MOTA	1924	CE	LYS	257		15.566	6.085	42.412	1.00 36.06	В
	ATOM	1925	NZ	LYS	257		15.142	6.972	41.303	1.00 38.19	В
15	ATOM	1926	С	LYS	257		14.408	9.497	46.777	1.00 34.33	В
	MOTA	1927	0	LYS	257		15.100	10.227	46.074	1.00 35.94	В
•	MOTA	1928	N	ILE	258		14.618	9.345	48.074	1.00 31.24	В
	MOTA	1929	CA	ILE	258		15.677	10.066	48.747	1.00 27.10	В
	ATOM	1930	CB	ILE	258		15.077	10.988	49.842	1.00 28.34	В
20	ATOM	1931		ILE	258		16.181	11.791	50.516	1.00 26.47	B
	ATOM	1932		ILE	258		14.021	11.949	49.203	1.00 27.71	В
	ATOM	1933		ILE	258		13.168	12.703	50.214	1.00 25.91	В.
	ATOM	1934	c	ILE	258		16.695	9.136	49.382	1.00 24.38	В.
	ATOM	1935	ŏ	ILE	258		16.386	8.400	50.314	1.00 22.26	В
25	ATOM	1936	N	GLY	259		17.917	9.182	48.872	1.00 22.20	
25	ATOM	1937	CA	GLY	259		18.975		49.422		В
								8.359		1.00 22.93	В
	MOTA	1938	C	GLY	259		20.055	9.163	50.135	1.00 22.70	В
	MOTA	1939	0	GLY	259	•	20:561	10.161	49.609	1.00 21.85	В
30	ATOM	1940	N	LYS	260		20.410	8.731	51.339	1.00 21.39	· В
30	ATOM	1941	CA	LYS	260		21.441	9.412	52.112	1.00 21.77	В
	MOTA	1942	CB	LYS	260		20.834	10.042	53.411	1.00 20.00	В
	MOTA	1943	CG	LYS	260		21.805	10.848	54.262	1.00 17.18	В
	MOTA	1944	CD	LYS	260		21.119	11.342	55.534	1.00 16.09	В
25	MOTA	1945	CE	LYS	260		22.049	12.181	56.417	1.00 16.97	В
35	MOTA	1946	NZ	LYS	260		21.341	12.724	57.641	1.00 15.85	В
•	MOTA	1947	C	LYS	260		22.545	8.419	52.469	1.00 21.92	В
	MOTA	1948	0	LYS	260		22.284	7.303	52.938	1.00 22.32	В
	MOTA	1949	N	LEU	261		23.780	8.837	52.236	1.00 19.52	В
40	ATOM	1950	CA	LEU	261		24.932	8.009	52.520	1.00 17.05	В
40	MOTA	1951	CB	LEU	261		25.693	7.741	51.235	1.00 14.85	В
	MOTA	1952	CG	LEU	261		27.111	7.236	51.385	1.00 14.96	В
	MOTA	1953	CD1	LEU	261		27.114	5.939	52.165	1.00 12.47	В.
	MOTA	1954		LEU	261		27.730	7.054	50.019	1.00 12.11	В
	MOTA	1955	C	LEU	261		25.828	8.720	53.519	1.00 17.96	В
45	ATOM	1956	0	LEU	261		26.258	9.850	53.284	1.00 16.25	В
	MOTA	1957	N	ASN	262		26.099	.8.063	54.643	1.00 18.12	В
	ATOM	1958	CA	ASN	262		26.970	8.640	55.670	1.00 18.04	В
	ATOM	1959	ÇВ	ASN	262		26.336	8.512	57.080	1.00 15.45	В
	ATOM	1960	CG.	ASN	262		24.943	9.103	57.152	1.00 17.34	В
50	ATOM	1961		ASN	262		23.957	8.381	57.282	1.00 17.52	В
•	ATOM	1962		ASN	262		24.855	10.420	57.070	1.00 17.02	В
	ATOM	1963	C	ASN	262		28.327	7.929	55.664	1.00 18.26	В
	ATOM	1964	ŏ	ASN	262		28.399	6.697	55.735	1.00 16.20	В
	MOTA	1965	N	LEU	263		29.394	8.717	55.564	1.00 18.04	
55	ATOM	1966	CA	LEU	263		30.759	8.200	55.560		В
"	ATOM		CB							1.00 17.90	В
		1967		LEU	263		31.482	8.723	54.339	1.00 15.70	В
	MOTA	1968	CG		263		30.717	8.283		1.00 17.05	В
	ATOM	1969		LEU	263		31.255	8.961	51.853	1.00 16.38	В
60 -	MOTA	1970		LEU	263		30.812	6.754	52.929	1.00 18.46	В
OU '	MOTA	1971	Ç	LEU	263		31:411	8.688	56.849	1.00 18.79	В
	ATOM	1972	0	LEU	263		31.712	9.873	56.992	1.00 20.38	В
	ATOM	1973	N	VAL	264		31.614	7.774	57.794	1.00 18.49	В
	ATOM	1974	CA	VAL	264		32.183	8.128	59.093	1.00 18.30	В
	ATOM	1975	CB	VAL	264		31.335	7.529	60.228	1.00 18.68	В
65	MOTA	1976	CG1	VAL	264		31.752	8.115	61.561	1.00 17.56	В
	ATOM	1977	CG2	VAL	264		29.858	7.772	59.955	1.00 21.14	В
	MOTA	1978	С	VAL	264		33.627	7.696	59.333	1.00 19.31	В
	ATOM	1979	ō	VAL	264		33.952	6.513	59.210	1.00 19.80	В
	ATOM	1980	N	ASP	265		34.478	8.667	59.680	1.00 17.61	В
70	ATOM	1981	CA	ASP	265		35.880	8.419	59.995	1.00 17.01	В
-	MOTA	1982	СВ	ASP	265		36.771	9.484	59.355	1.00 13.38	В
	MOTA	1983	CG	ASP	265		38.258	9.279	59.658	1.00 14.42	
	MOTA	1984		ASP	265		38.583				В
	ALON	A 704	001	VOL	203		JU. JUJ	8.741	60.736	1.00 19.48	В

										_
	MOTA	1985		ASP	265	39.110	9.677	58.832	1.00 16.17	В
	ATOM	1986	C	ASP	265	35.971	8.507	61.528	1.00 15.62	В
	MOTA	1987	0	ASP	265	36.119	9.593	62.086	1.00 17.19	В
5	ATOM	1988	N	LEU	266	35.891.	7.367	62.205	1.00 13.53	В
5	MOTA	1989	CA	LEU	266	35.930	7.357	63.666	1.00 12.99	В
	ATOM .	1990	CB	LEU	266	35.555	5.913	64.239	1.00 9.90	В
	MOTA	1991	CG	LEU	266	34.172	5.339	63.898	1.00 12.88	В
	MOTA	1992		LEU	266	34.070	3.881	64.374	1.00 12.44	В
10	MOTA	1993		LEU	266	33.088		64.542	1.00 11.19	В
10	MOTA	1994	C	LEU	266	37.277	7.783	64.240	1.00 11.25	В
	ATOM	1995	0	LEU	266	38.274	7.867	63.532	1.00 7.77	B
	MOTA	1996	N	ALA	267	37.263	8.059	65.539	1.00 10.58	В
	MOTA	1997	CA	ALA	267	38.453	8.422	66.284	1.00 13.04	В
. ~	MOTA	1998	CB	ALA	267	38.057	9.029	67.634	1.00 11.27	В
15	ATOM	1999	С	ALA	267	39.221	7.125	66.507	1.00 14.13	В
	MOTA	2000	0	ALA	267 .	38.610	6.077	66.718	1.00 16.34	В
	MOTA	2001	N	GLY	268	40.546	7.190	66.475	1.00 14.85	j B
	ATOM	2002	CA	GLY	268	41.347	5.999	66.688	1.00 17.83	В
	ATOM	2003	С	GLY	268	40.934	5.198	67.909	1.00 20.15	В
20	MOTA	2004	0	GLY	268	40.663	5.760	68.978	1.00 21.52	В
	ATOM	2005	N	SER	269	. 40.918	3.878	67.773	1.00 20.60	В
	ATOM ·	2006	CA	SER	269	40.500	3.017	68.878	1.00 23.05	В
	MOTA	2007	CB	SER	269	39.929	1.721	68.324	1.00 20.23	В
~ -	ATOM	2008	OG	SER	269	40.842	1.099	67.442	1.00 17.43	В
25	MOTA	2009	С	SER	269	41.546	2.678	69.941	1.00 26.49	· B
	ATOM	2010	0	SER	269	41.227	1.969	70.903	1.00 27.04	. В
	MOTA	2011	N	GLU	270	42.775	3.171	69.781	1.00 29.47	В
	ATOM	2012	CA	GLU	270	43.848	2.887	70.743	1.00 32.95	В
	ATOM	2013	CB	GLU	270	45.234	3.432	70.210	1.00 32.65	В
30	MOTA	2014	CG	GLU	270	45.405	4.968	70.193	1.00 30.27	В
	MOTA	2015	CD	GLU	270	44.822	5.656	68.963	1.00 30.89	В
	MOTA	2016	OE1	GLU	270	44.879	6.908	68.911	1.00 32.19	В
	MOTA	2017	OE2	GLU	270.	44.315	4.961	68.052	1.00 28.80	В
	ATOM	2018	С	GLU	270	43.560	3.472	72.129	1.00 36.87	В
35	ATOM	2019	0	GLU	270	43.380	4.681	72.277	1.00 39.21	В
	ATOM	2020	N	ASN	271	43.503	2.613	73.143	1.00 40.27	В
	ATOM	2021	CA	ASN	271	43.238	3.062	74.515	1.00 42.68	В
	ATOM	2022	СВ	ASN	271	42.196	2.131	75.222	1.00 43.15	В
	ATOM	2023	CG	ASN	271	40.798	2.244	74.621	1.00 45.39	В
40	ATOM	2024		ASN	271	40.230	3.337	74.540	1.00 46.39	В
	ATOM	2025	ND2		271	40.232	1.109	74.210	1.00 43.39	В
	ATOM	2026	C	ASN	271	44.528	3.093	75.331	1.00 43.55	В
	ATOM	2027	Ō	ASN	271	45.603	2.746	74.833	1.00 43.93	В
	MOTA	2028	N	ASN	287	41.588	11.864	79.666	1.00 44.94	В
45	MOTA	2029	CA	ASN	287	40.716	12.252	78.558	1.00 45.22	В
	ATOM	2030	СВ	ASN	287	41.514	13.086	77.476	1.00 48.29	В
	ATOM	2031	CG	ASN	287	42.261	14.276	78.074	1.00 50.68	В
	MOTA	2032	OD1		287	43.249	14.106	78.796	1.00 51.76	В
	MOTA	2033	ND2	ASN	287	41.791	15.488	77.774	1.00 51.75	В
50	MOTA	2034	С	ASN	287	40.091	11.016	77.897	1.00 42.90	В
	ATOM	2035	0	ASN	287	40.787	10.182	77.315	1.00 42.06	В
	MOTA	2036	N	ILE	288	38.771	10.914	77.995	1.00 40.12	В
	ATOM	2037	CA	ILE	288	38.034	9.794	77.424	1.00 36.62	В
	MOTA	2038	CB	ILE	288	37.110	9.146	78.479	1.00 37.65	В
55	MOTA	2039	CG2	ILE	288	37.911	8.154	79.325	1.00 38.70	В
	MOTA	2040	CG1	ILE	288	36.464	10.252	79.390	1.00 36.64	В
	MOTA	2041	CD1	ILE	288	35.583	11.252	78.657	1.00 36.28	В
	MOTA	2042	С	ILE	288	37.183	10.200	76.230	1.00 33.35	В
	ATOM	2043	0	ILE	288	36.763	11.356	76.100	1.00 34.53	. В
60	MOTA	2044	N	ASN	289	36.938	9.252	75.342	1.00 27.16	В
	MOTA	2045	CA	ASN	289	36.112	9.564	74.199	1.00 23.25	В
	ATOM	2046	СВ	ASN-	289	36.731	9.052	72.954	1.00 20.82	В
	ATOM	2047	CG	ASN	289	36.172	9.721	71.712	1.00 19.85	B
	ATOM	2048	OD1		289	36.929	10.208	70.878	1.00 19.66	. B
65	ATOM	2049	ND2		289	34.846	9.737	71.576	1.00 17.37	В
	ATOM	2050	C	ASN	289	34.763	8.912	74.459	1.00 20.79	В
	ATOM	2051	ō	ASN	289	34.553	7.735	74.170	1.00 18.65	В
	ATOM .	2052	N	GLN	290	33.863	9.694	75.042	1.00 19.57	В
	MOTA	2053	CA	GLN	290	32.537	9.216	75.379	1.00 19.29	В
70	ATOM	2054	CB.	GLN	290	31.678	10.366	75.901	1.00 19.26	В
	ATOM	2055	CG	GLN	290	30.278	9.942	76.312	1.00 19.65	В
	ATOM	2056	CD	GLN	290	30.265	8.891	77.423	1.00 20.79	В
	ATOM	2057	OE1		290	29.211	8.339	77.754	1.00 21.88	В
		- -			-					

	A'TOM'	2058	NE2	GLN	290	31.427	8:621	78.006	1.00 18.18	В
	MOTA	2059	C	GLN	290	31.830	8.538	74.214	1.00 18.80	В
	MOTA	2060	ŏ							
				GLN	290	31.199	7.502	74.397	1.00 17.47	В
5	MOTA	2061	N	SER	291	31.939	9.122	73.021	1.00 18.97	В
J	MOTA	2062	CA	SER	291	31.289	8.565	71.841	1.00 18.84	В
	ATOM	2063	CB	SER	291	31.326	9.565	70.646	1.00 19.15	В
	ATOM	2064	OG	SER	291	30.347	10.593	70.784	1.00 19.00	В
	ATOM	2065	С	SER	291	31.897	7.239	71.420	1.00 19.68	В
	MOTA	2066	Ō	SER	291	31.173	6.323	71.027	1.00 21.26	В
10	ATOM	2067	N	LEU	292	33.219	7.131	71.494	1.00 18.43	В
10	ATOM									
		2068	CA	LEU	292	33.872	5.888	71.128	1.00 17.73	В
	MOTA	2069	CB	LEU	292	35.361	6.070	71.140	1.00 15.77	В
•	ATOM	2070	CG	LEU	292	36.119	4.969	70.418	1.00 15.31	В
. ~	MOTA	2071	CD1	LEU	292 .	35.703	4.951	68.953	1.00 11.07	В
15	ATOM	2072	CD2	LEU	292	37.621	5.213	70.548	1.00 16.30	В
	MOTA	2073	С	LEU	292	33.461	4.827	72.159	1.00 19.37	В
	ATOM	2074	0	LEU	292	33.107	3.698	71.814	1.00 20.03	В
	ATOM	2075	N	LEU	293	33.504	5.219	73.430	1.00 19.01	В
	ATOM	2076	CA	LEU	293	33.137	4.357	74.531	1.00 18.18	В
20	MOTA	2077	CB	LEU	293					
20						33.194	5.140	75.819	1.00 16.50	В
	ATOM	2078	CG	LEU	293	34.193	4.752	76.903	1.00 18.80	В
	MOTA	2079		LEU	293	35.291	3.824	76.354	1.00 14.59	В,
	MOTA	2080	CD2	LEU	293	34.789	6.039	77.485	1.00 18.33	В
	MOTA	2081	С	LEU	293	31.724	3.828	74.326	1.00 20.79	·B
25	MOTA	2082	0	LEU	293	31.446	2.629	74.480	1.00 21.79	В
	ATOM	2083	N	THR	294	30.824	4.730	73.972	1.00 20.82	В
	ATOM	2084	CA	THR	294 .		4.348	73.785	1.00 21.70	В
	ATOM	2085	CB	THR	294	28.556	5.607	73.770	1.00 21.45	В
	MOTA	2086		THR	294	28.737	6.305	75.012		
30									1.00 20.05	В
50	MOTA	2087		THR	294	27.085	5.243	73.638	1.00 23.08	В
	MOTA	2088	C	THR	294	29.245	3.488	72.541	1.00 22.57	В
	MOTA	2089	0	THR	294	28.410	2.589	72.541	1.00 24.83	В
	ATOM	2090	N	LEU	295	30.028	3.726	71.492	1.00 22.48	В
~ -	ATOM	2091	CA	LEU	295	29.888	2.929	70.278	1.00 20.67	В
35	MOTA	-2092	CB	LEU	295	30.896	3.354	69.239	1.00 16.50	В
	MOTA	2093	CG	LEU	295	30.872	2.542	67.933	1.00 15.31	B
	ATOM	2094		LEU	295	29.480	2.540	67.301	1.00 9.83	В
	ATOM	2095		LEU		31.901				
								66.996	1.00 13.69	В
40	MOTA	2096	C	LEU	295	30.072	1.453	70.614	1.00 21.75	В
40	MOTA	2097	0	LEU	295	29.261	0.620	70.222	1.00 22.82	В
	ATOM	2098	N	GLY	296	31.141	1.141	71.345	1.00 22.87	В
	MOTA	2099	CA	GLY	296	31.402	-0.230	71.753	1.00 21.35	В
	ATOM	2100	С	GLY	296	30.318	-0.785	72.668	1.00 20.58	В
	ATOM	2101	0	GLY	296	29.960	-1.950	72.566	1.00 22.84	В
45	MOTA	2102	N	ARG	297	29.782	0.034	73.562	1.00 19.00	В
	ATOM	2103	CA	ARG	297	28.735	-0.441	74.462	1.00 18.91	В
	ATOM	2104	СВ	ARG	297	28.530	0.539	75.601	1.00 17.91	B
	MOTA	2105	CG	ARG	297	29.645	0.523	76.596		
	ATOM	2106	CD.		297				1.00 17.55	В
50				ARG		29.622	1.775	77.433	1.00 21.12	В
50	MOTA	2107	NE	ARG	297	30.783	1.860	78.311	1.00 20.84	В
	MOTA	2108	CZ	ARG	297	31.212	2.987	78.862	1.00 19.95	В
	MOTA	2109	NH1		297	30.567	4.118	78.614	1.00 19.89	В
	MOTA	2110	NH2	ARG	297	32.274	2.982	79.661	1.00 15.55	В
	ATOM	2111	С	ARG	297	27.419	-0.662	73.733	1.00 18.05	В
55	ATOM	2112	0	ARG	297	26.581	-1.440	74.177	1.00 18.18	В
	MOTA	2113	N	VAL	298	27.235	0.035	72.618	1.00 19.06	В
	ATOM	2114	CA	VAL			-0.106		1.00 17.97	B
	ATOM	2115	CB	VAL	298	25.816	1.111	70.885	1.00 15.95	
	MOTA	2116		VAL	298					В.
60 -						24.691	0.843	69.899	1.00 13.08	В
UU	MOTA	2117		VAL	298	25.507	2.350	71.710	1.00 14.44	В
	MOTA	2118	С	VAL	298	26.140	-1.377	70.985	1.00 19.67	В
	MOTA	2119	0	VAL	298	25.153	-2.075	70.749	1.00 21.91	В
	MOTA	2120	N	ILE	299	27.356	-1.686	70.544	1.00 19.47	В
	MOTA	2121	CA	ILE	299	27.570	-2.879	69.736	1.00 21.25	В
65	MOTA	2122	CB	ILE	299	28.973	-2.830	69.068	1.00 21.35	В
	MOTA	2123		ILE	299	29.354	-4.192	68.502	1.00 19.14	В
	ATOM	2124	CG1		299	28.950	-1.752	67.932		
	ATOM	2125							1.00 19.67	В
				ILE	299	30.316	-1.238	67.523	1.00 19.64	В
70	MOTA	2126	C	ILE	299	27.399	-4.122	70.610	1.00 22.50	В
70	MOTA	2127	0	ILE	299	26.774	-5.102	70.206	1.00 21.52	В
	MOTA	2128	N	THR	300	27.936	-4.057	71.821	1.00 23.04	В
	MOTA	2129	CA.	THR	300	27.827	-5.153	72.763	1.00 23.72	В
	MOTA	2130	CB	THR	300	28.521	-4.787	74.068	1.00 23.18	В

	MOTA	2131	001	THR	300	29.923	-4.646	73.811	1.00 21.92	В
	MOTA	2132	CG2		300	28.284	-5.841	75.138	1.00 17.93	. В
	MOTA	2133	С	THR	300	26.353	-5.447	73.020	1.00 27.59	В
-	MOTA	2134	0	THR	300	25.878	-6.563	72.787	1.00 27.46	В
5	MOTA	2135	N	ALA	301	25.626	-4.438	73.480	1.00 29.03	В
	ATOM .	2136	CA	ALA	301	24.206	-4.600	73.754	1.00 30.76	В
	ATOM	2137	СВ	ALA	301	23.598	-3.262	74.139	1.00 31.16	В
	ATOM	2138	Č	ALA	301	23.437	-5.196	72.573	1.00 32.99	
										В
10	ATOM	2139	0	ALA	301	22.545		72.772	1.00 35.01	В
10	MOTA	2140	N	LEU	302	23.770	-4.780	71.351	1.00 34.50	В
	ATOM	2141	CA	LEU	302	23.088	-5.279	70.152	1.00 34.70	· В
	MOTA	2142	CB	LEU	302	23.440	-4.425	68.943	1.00 35.01	В
	ATOM .	2143	CG	LEU	302	22.840	-2.999	68.895	1.00 35.55	В
	ATOM	2144		LEU	302	23.474	-2.227	67.759	1.00 36.40	В
15		2145								
13	MOTA	-		LEU	302	21.334	-3.063	68.714	1.00 33.89	В
	MOTA	2146	С	LEU	302	23.451	-6.721	69.855	1.00 35.87	, B
	ATOM	2147	. 0	LEU	302	22.590	-7.547	69.549	1.00 36.50	В
•	ATOM	2148	N	VAL	303	24.742	-7.008	69.941	1.00 36.97	В
	MOTA	2149	CA	VAL	303	25.271	-8.339	69.691	1.00 36.81	В
20	ATOM	2150	CB	VAL	303	26.818	-8.289	69.707	1.00 36.26	В
	MOTA	2151	CG1		303	27.402	-9.658	69.961		
									1.00 35.12	В
	ATOM	2152	CG2		303	27.316	-7.726	68.384	1.00 35.06	В
	MOTA	2153	С	VAL	303	24.757	-9.359	70.711	1.00 38.19	В
~ "	ATOM	2154	0	VAL	303	24.495	-10.506	70.368	1.00 39.57	В
25	ATOM	2155	N	GLU	304	24.597	-8.928	71.957	1.00 39.43	В
	ATOM	2156	CA	GLU	304	24.129	-9.796	73.032	1.00 40.38	В
	MOTA	2157	СВ	GLU	304	24.768	-9.359	74.350	1.00 41.03	В
	MOTA	2158	CG	GLU				74.347		
					304	26.290	-9.464		1.00 42.14	B
20	MOTA	2159	CD	GLU	304	26.889	-9.210	75.713	1.00 43.89	В
30	MOTA	2160		GLU	304	28.116	-9.390	75.879	1.00 42.77	В
	ATOM	2161	OE2	GĽU	.304	26.127	-8.827	76.625	1.00 45.66	В
	MOTA	2162	С	GLU	304	22.612	-9.817	73.179	1.00 41.20	В
	ATOM	2163	0	GLU	304 .	22.071	-10.477	74.062	1.00 39.68	В
	ATOM	2164	N	ARG	305	21.932	-9.088	72.305	1.00 44.11	В
35	ATOM	2165	CA	ARG	305					
<i></i>						20.474	-9.004	72.310	1.00 46.91	В.
	ATOM	2166	CB	ARG	305	19.835	-10.408	71.997	1.00 48.72	В
	· ATOM	2167	CG	ARG	305	20.520	-11.222	70.897	1.00 52.86	В
	ATOM	2168	CD	ARG	305	20.686	-10.461	69.579	1.00 56.32	В
	MOTA	2169	NE	ARG	305	21.395	-11.268	68.582	1.00 59.70	В
40	MOTA	2170	CZ	ARG	305	21.970	-10.782	67.483	1.00 61.81	B
	ATOM	2171		ARG	305	21.926	-9.479	67.221	1.00 61.95	В
	MOTA	2172		ARG	305	22.605				
							-11.601	66.649	1.00 61.81	В
	MOTA	2173	C	ARG	305	19.890	-8.469	73.620	1.00 47.13	В
45	MOTA	2174	0	ARG	305	18.784	-8.840	73.996	1.00 48.14	В
45	MOTA	2175	N	THR	306	20.621	-7.599	74.311	1.00 48.36	В
	MOTA	2176	CA	THR	306	20.135	-7.027	75.568	1.00 49.45	В
	MOTA	2177	CB	THR	306	21.275	-6.367	76.356	1.00 49.08	В
	ATOM	2178		THR	306	22.429	-7.214	76.326	1.00 49.36	В
	ATOM	2179								
50				THR	306	20.862	-6.155	77.802	1.00 48.92	В
J U	MOTA	2180	C	THR	306	19.066	-5.972	75.262	1.00 50.64	В
	MOTA	2181	0	THR	306	19.275	-5.091	74.428	1.00 51.81	В
	MOTA	2182	N	PRO	307	17.910	-6.044	75.942	1.00 51.76	В
	ATOM	2183	CD	PRO	307	17.651	-6.959	77.068	1.00 52.91	В
	ATOM	2184	CA	PRO	307	16.779	-5.119	75.761	1.00 52.01	В
55	ATOM	2185	CB	PRO	307	15.945	-5.358	76.995	1.00 52.53	B
	ATOM	2186	CG	PRO	307	16.158	-6.818	77.257		
									1.00 53.28	В
	ATOM	2187	C	PRO	307	17.124	-3.638	75.585	1.00 51.42	В
	MOTA	2188	0	PRO	307	16.624	-2.983	74.664	1.00 51.33	В
~ ^	ATOM	2189	N	HIS	308	17.973	-3.115	76.466	1.00 49.88	В
60	MOTA	2190	CA	HIS	308	18.359	-1.711	76.410	1.00 47.29	В
	ATOM	2191	СB	HIS	308	18.432	-1.141	77.832	1.00 50.27	В
	ATOM	2192	CG	HIS	308	18.812	0.306	77.877	1.00 54.50	В
	ATOM	2193		HIS						
					308	19.992	0.909	78.158	1.00 55.48	В.
65	MOTA	2194		HIS	308	17.931	1.318	77.559	1.00 55.94	В
UJ	MOTA	2195		HIS	308	18.552	2.482	77.641	1.00 56.20	В
	MOTA	2196	NE2	HIS	308	19.804	2.262	78.003	1.00 56.35	В
	MOTA	2197	С	HIS	308	19.685	-1.445	75.690	1.00 43.71	В
	MOTA	2198	Ō	HIS	308	20.709	-2.061	75.991	1.00 43.17	В
	ATOM	2199	N	VAL	309	19.649	-0.517	74.737	1.00 39.63	В
70	MOTA	2200	CA	VAL	309					
, 0						20.829	-0.117	73.964	1.00 34.96	В
	ATOM	2201	CB	VAL	309	20.561	-0.206	72.449	1.00 34.96	₿
	MOTA	2202		VAL	309	21.858	0.013	71.675	1.00 34.27	В
	MOTA	2203	CG2	VAL	309	19.934	-1.548	72.114	1.00 32.68	B
				•						

	ATOM	2204	С	VAL	309	21.086	1.344	74.336	1.00 31.77	. В
	ATOM	2205	0	VAL	309	20.237	2.204	74.102	1.00 30.77	В
	ATOM	2206	N	PRO	310	22.266	1.642	74.906	1.00 29.55	В
5	ATOM	2207	CD	PRO	310	23.347	0.670	75.171	1.00 27.65	В
3	MOTA	2208	CA	PRO	310	22.652	2.997	75.335	1.00 29.03	В
	ATOM	2209	CB	PRO	310	23.856	2.732	76.230	1.00 29.20	В
	ATOM ATOM	2210 2211	CG	PRO PRO	310 310	24.518 22.949	1.555 4.064	75.539	1.00 27.40 1.00 28.13	В
	MOTA	2212	0	PRO	310	23.960	4.760	74.268 74.357	1.00 27.93	B
10	ATOM	2213	N	TYR	311	22.064	4.198	73.284	1.00 27.73	В
	ATOM	2214	CA	TYR	311	22.217	5.175	72.203	1.00 28.46	В
	ATOM	2215	CB	TYR	311	20.949	5.195	71.291	1.00 29.00	В
	MOTA	2216	CG	TYR	311	20.724	3.960	70.450	1.00 32.30	В
15	MOTA	2217		TYR	311	21.600	3.631	69.413	1.00 32.05	В
.15	MOTA	2218		TYR	311	21.393	2.492	68.628	1.00 34.37	В
	ATOM ATOM	2219	CD2	TYR	311	19.627	3.119	70.686	1.00 31.31	. В
	ATOM	2220 2221	CE2 CZ	TYR TYR	311 311	19.411 20.299	1.979 1.669	69.908 68.882	1.00 32.07	B B
	ATOM	2222	ОН	TYR	311	20.120	0.531	68.122	1.00 35.43	В
20	MOTA	2223	c	TYR	311	22.458	6.611	72.678	1.00 28.67	, B
	MOTA	2224	0	TYR	311	23.343	7.296	72.177	1.00 27.07	В
	MOTA	2225	Ŋ	ARG	312	21.652	7.059	73.635	1.00 29.15	В
	MOTA	2226	CA	ARG	312	21.716	8.425	74.143	1.00 29.95	В
25	ATOM	2227	CB	ARG	312	20.481	8.724	74.961	1.00 32.31	В
23	MOTA MOTA	2228 2229	CD	ARG ARG	312 312	19.189	8.626 8.529	74.196	1.00 36.65	В
	ATOM	2230	NE	ARG	312	18.046 16.862	7.919	75.169 74.577	1.00 40.81	B B
	ATOM	2231	CZ	ARG	312	15.951	7.251	75.278	1.00 45.73	В
	MOTA	2232		ARG	312	16.100	7.108	76.597	1.00 44.15	. B
30	MOTA	2233	NH2	ARG	312	14.888	6.737	74.664	1.00 45.91	В
	MOTA	2234	С	ARG	312	22.926	8.811	74.969	1.00 28.83	В
	MOTA	2235	0	ARG	312	23.104	9.991	75.276	1.00 29.69	В
	ATOM	2236	N	GLU	313	23.755	7.843	75.340	1.00 26.62	В
35	MOTA MOTA	2237 2238	CA CB	GLU	313 313	24.917	8.160	76.153	1.00 22.31	В
55	MOTA	2239	CG	GLU	313	25.419 24.550	6.929 6.521	76.814 77.994	1.00 22.37	B B
	ATOM	2240	CD	GLU	313	24.871	5.136	78.554	1.00 26.13	В
	ATOM	2241	OE1		313	26.060	4.823	78.755	1.00 27.91	В
40	MOTA	2242	OE2	GLU	313	23.926	4.365	78.813	1.00 27.77	В
40	MOTA	2243	С	GLU	313	26.031	8.873	75.403	1.00 21.16	В
	MOTA	2244	0	GLU	313	27.096	9.122	75.963	1.00 21.76	В
	MOTA	2245	N	SER	314	25.789	9.222	74.144	1.00 18.52	В
	MOTA MOTA	2246 2247	CA CB	SER SER	314 314	26.796 27.966	9.935 8.992	73.375 72.968	1.00 19.81 1.00 20.10	B B
45	ATOM	2248	QG	SER	314	27.731	8.382	71.710	1.00 19.29	В
-	MOTA	2249	Č	SER	314	26.206	10.583	72.130	1.00 20.60	В
	MOTA	2250	Ο.	SER	314	25.198	10.126	71.597	1.00 19.90	В
	ATOM	2251	N	LYS	315	26.854	11.654	71.676	1.00 20.92	В
50	MOTA	2252	CA	LYS	315	26.412	12.395	70.504	1.00 20.48	В
50	MOTA	2253	CB	LYS	315	27.264	13.689	70.329	1.00 20.26	В
	MOTA MOTA	2254 2255	CG	LYS	315 315	27.318 25.936	14.572 14.893	71.556 72.074	1.00 19.73	B B
	ATOM	2256	CE	LYS	315	25.984	15.989	73.129	1.00 23.41	B
	ATOM	2257	NZ	LYS	315	26.408	17.293	72.528	1.00 26.09	В.
55	MOTA	2258	С	LYS	315	26.513	11.560	69.239	1.00 19.78	В
	MOTA	2259	0	LYS	315	25.626	11.614	68.373	1.00 20.29	В
	MOTA	2260	N	LEU	316	27.598	10.796	69.130	1.00 17.65	В
	MOTA	2261	CA	LEU	316	27.808	9.962	67.955	1.00 17.80	В
60	MOTA MOTA	2262 2263	CB CG	LEU	316 316	29.209	9.245	68.013	1.00 16.46	В
00	MOTA	2264		LEU	316	29.602 29.683	8.339 9.151	66.775 65.507	1.00 15.01 1.00 14.12	B B
	ATOM	2265		LEU.	316	30.937	7.695	67.030	1.00 17.53	В
	MOTA	2266	C	LEU	316	26.698	8.926	67.798	1.00 17.14	В
	MOTA	2267	0	LEU	316	26.060	8.854	66.742	1.00 17.17	В
65	ATOM	2268	N	THR	317	26.462	8.137	68.844	1.00 17.69	В
	MOTA	2269	CA	THR	317	25.439	7.106	68.777	1.00 19.04	В
	MOTA	2270	CB	THR	317	25.525	6.124	69.966	1.00 21.44	В
	MOTA	2271	0G1		317	25.617	6.848	71.198	1.00 21.96	В
70	MOTA MOTA	2272 2273	CG2 C	THR	317 317	26.743 24.031	5.206 7.659	69.804 68.659	1.00 21.41	В
. •	MOTA	2274	ò	THR	317	23.155	6.990	68.130	1.00 18.09	B B
	ATOM	2275	N .	ARG	318	23.800	8.877	69.134	1.00 19.16	В
	MOTA	2276	CA	ARG	318	22.469	9.460	68.986	1.00 20.49	В

	MOTA	2277	СВ	ARG	318	22.283	10 654	69.927	1.00 22.85	В
	MOTA	2278	CG	ARG	318	22.155	10.218	71.387	1.00 28.27	В
	MOTA	2279	CΩ	ARG	318	21.942	11.375	72.318	1.00 31.62	В
_	ATOM	2280	NE	ARG	318	20.929	12.277	71.788	1.00 39.60	В
5	MOTA	2281	CZ	ARG	318	20.361	13.261	72.479	1.00 40.99	В
	MOTA	2282	NH1	ARG	318	20.703	13.474	73.746	1.00 41.19	. в
	MOTA	2283		ARG	318	19.454	14.034	71.894	1.00 41.05	B
								67.525		
	MOTA	2284	C	ARG	318	22.288	9.873		1.00 20.16	В
10	MOTA	2285	0	ARG	318	21.237		66.929	1.00 21.26	В
10	ATOM	2286	N	ILE	319	23.332	10.435	66.932	1.00 18.27	В
	MOTA	2287	CA	ILE	319	23.255	10.843	65.539	1.00 18.18	· B
	ATOM	2288	CB	ILE	319	24.505	11.665	65.132	1.00 17.80	В
	MOTA	2289		ILE	319		11.913	63.619	1.00 17.11	В
	MOTA			ILE	319	24.561	13.006	65.928	1.00 17.07	B
15										
IJ	MOTA	2291		ILE	319	25.901	13.727	65.838	1.00 14.30	В
	MOTA	2292	C	ILE	319	23.134	9.663	64.550	1.00 18.77	В
	MOTA	2293	. 0	ILE	319	22.397	9.753	63.569	1.00 16.28	·B
	MOTA	2294	N	LEU	320	23.860	8.571	64.808	1.00 18.72	• В
	MOTA	2295	CA	LEU	320	23.874	7.415	63.905	1.00 18.52	В
20	MOTA	2296	CB	LEU	320	25.323	7.003	63.621	1.00 14.27	В
	ATOM	2297	CG	LEU	320	26.321	8.000	63.025	1.00 16.38	В
	ATOM	2298		LEU	320	27.707	7.354	63.023		
									1.00 13.61	В
	MOTA	2299		LEU	320	25.905	8.426	61.605	1.00 14.32	В
05	MOTA	2300	C	LEU	320	23.113	6.159	64.354	1.00 21.16	В
25	MOTA	2301	0	LEU	320	23.308	5.087	63.780	1.00 21.77	В
	MOTA	2302	N	GLN	321	22.249	6.277	65.357	1.00 22.79	. В
	MOTA	2303	CA	GLN	321	21.519	5.114	65.848	1.00 25.68	В
	MOTA	2304	CB	GLN	321	20.531	5.524	66.954	1.00 28.52	В
	MOTA	2305	CG	GLN	321	19.448	6.490	66.535	1.00 32.15	В
30	MOTA									
50		2306	CD	GLN	321	18.539	6.843	67.700	1.00 35.99	В
	MOTA	2307		GLN	321	17.953	5.954	68.332	1.00 33.89	В
	MOTA	2308	NE2	GLN	321	18.417	8.144	67.997	1.00 36.73	В
	MOTA	2309	С	GLN	321.	20.790	4.254	64.813	1.00 25.53	В
	ATOM	2310	0	GLN	321	20.625	3.056	65.029	1.00 25.73	В
35	ATOM	2311	N	ASP	322	20.353	4.837	63.701	1.00 26.46	В.
	ATOM	2312	CA	ASP	322	19.659	4.040	62.695	1.00 28.33	В
	MOTA	2313	СВ	ASP	322	18.913	4.934	61.681	1.00 29.02	В
	MOTA	2314	CG	ASP	322	17.894	4.152	60.847	1.00 30.51	В
4'0	MOTA	2315	OD1	ASP	322	17.880	4.308	59.604	1.00 31.51	В
40	MOTA	2316	OD2	ASP	322	17.100	3.384	61.434	1.00 29.46	В
	MOTA	2317	С	ASP	322	20.661	3.152	61.959	1.00 29.44	В
	MOTA	2318	0	ASP	322	20.284	2.195	61.280	1.00 29.55	В
	MOTA	2319	N	SER	323	21.943	3.480	62.095	1.00 29.59	В
	MOTA	2320	CA	SER	323	22.999	2.705	61.458	1.00 28.78	
45										В
47	MOTA	2321	CB	SER	323	24.172	3.594	61.165	1.00 27.31	В
	MOTA	2322	OG	SER	323	23.845	4.545	60.178	1.00 26.34	В
	MOTA	2323	С	SER	323 .	23.453	1.519	62.322	1.00 29.30	В
	MOTA	2324	0	SER	323	24.234	0.687	61.875	1.00 28.51	В
	MOTA	2325	N	LEU	324	22.967	1.445	63.558	1.00 30.19	В
50	ATOM	2326	CA	LEU	324	23.338	0.354	64.451	1.00 30.51	В
	ATOM	2327	СВ	LEU	324	24.110	0.893	65.662	1.00 30.62	В
	ATOM	2328	CG	LEU	324	25.577	1.365	65.474	1.00 29.76	В
				LEU						
	MOTA	-2329			324	25.670	2.412	64.401	1.00 31.76	В
e e	MOTA	2330		LEU	324	26.085	1.928	66.775	1.00 28.62	В
55	MOTA	2331	С	LEU	324	22.113	-0.419	64.927	1.00 31.44	В
	MOTA	2332	0	LEU	324	21.611	-0.184	66.026	1.00 32.71	В
	MOTA	2333	N	GLY	325	21.642	-1.347	64.095	1.00 31.87	В
	MOTA	2334	CA	GLY	325	20.479	-2.148	64.444	1.00 30.03	В
	MOTA	2335	Ċ.	GLY	325	19.190	-1.440	64.082	1.00 29.89	В
60										
UU	MOTA	2336	0	GLY	325	18.160	-1.636	64.727	1.00 29.38	В
	MOTA	2337	N	GLY	326	19.253	-0.614	63.042	1.00 29.59	В
	MOTA	2338	CA	GLY	326	18.092	0.139	62.603	1.00 27.99	В
	MOTA	2339	С	GLY	326	17.706	-0.236	61.193	1.00 27.84	В
	MOTA	2340	0	GLY	326	17.896	-1.378	60.811	1.00 28.56	В
65	MOTA	2341	N	ARG	327	17.197	0.719	60.418	1.00 26.60	В
	ATOM	2342	CA	ARG	327	16.763	0.456	59.046	1.00 27.36	
										В
	MOTA	2343	CB	ARG	327	15.451	1.234	58.745	1.00 30.55	В
	MOTA .	2344	CG	ARG	327	14.534	1.451	59.943	1.00 34.58	В
70	MOTA	2345	CD	ARG	327	13.775	0.198	60.367	1.00 40.44	В
70	MOTA	2346	NE	ARG	327	12.359	0.271	60.014	1.00 43.41	В
	MOTA	2347	CZ	ARG	327	11.898	0.209	58.768	1.00 47.99	В
	MOTA	2348		ARG	327	12.741	0.071	57.751	1.00 49.86	В
	ATOM	2349		ARG	327	10.592	0.285	58.535	1.00 48.98	В
			*****		J	24.332	V.20J	20.223	2.00 40.90	5

	MOTA	2350	С	ARG	327	1	7.796	0.811	57.967	1.00	27.20	В
	ATOM	2351	0	ARG	327		7.521	0.680	56.775	1 00	27.07	В
	•											
	MOTA	2352	N	THR	328		8.977	1.257	58.379		26.89	В
-	ATOM	2353	CA	THR	328	2	20.028	1.646	57.441	1.00	25.49	В
5	MOTA	2354	CB	THR	328	2	20.870	2.813	58.024	1.00	27.20	В
	ATOM	2355	OG1		328		0.024	3.944	58.252		29.46	В
	MOTA	2356	CG2		328		1.992	3.210	57.072		26.15	В
•	ATOM	2357	С	THR	328	2	0.974	0.492	57.125	1.00	24.96	В
	ATOM	2358	0	THR	328	2	1.238	-0.346	57.984	1.00	24.98	В
10	MOTA	2359	N	ARG	329		1.465	0.431	55.890		23.74	В
10												
	MOTA	2360	CA	ARG	329		2.426	-0.610	55.543		24.57	В
	ATOM	2361	CB	ARG	329	2	2.551	-0.842	54.014	1.00	26.29	В
	ATOM	2362	CG	ARG	329	2	3.421	-2.071	53.721	1.00	31.07	В
	MOTA	2363	CD	ARG	329		4.277	-1.980	52.461		34.15	В
.15		2364										
.13	MOTA		NE	ARG	329		3.590	-2.447	51.259		37.59	В
	MOTA	2365	CZ	ARG	329	2	4.217	-2.885	50.168	1.00	38.17	В
	MOTA	2366	NH1	ARG	329	2	5.547	-2.923	50.124	1.00	38.35	В
	ATOM	2367	NH2	ARG	329		3.513	-3.284	49.119	1 00	36.37	В
	ATOM	2368	c	ARG	329		3.761	-0.102	56.061			
20											22.51	В
20	MOTA	2369	0	ARG	329		4.174	1.012	55.741	1.00	21.91	В
	MOTA	2370	N	THR	330	2	4.431	-0.919	56.856	1.00	21.40	В
	MOTA	2371	CA	THR	330	2	5.704	-0.529	57.433	1.00	21.18	В
	ATOM	2372	CB	THR	330		5.610	-0.435	58.971		20.58	В.
25	MOTA	2373		THR	330		4.666	0.581	59.317		22.60	В
25	MOTA	2374	CG2	THR	330	2	6.962	-0.099	59.581	1.00	17.89	В
	MOTA	2375	С	THR	330	2	6.837	-1.471	57.085	1.00	21.32	В
	ATOM	2376	ō	THR	330		6.673	-2.691	57.001		19.41	В
						_						
	MOTA	2377	N	SER	331		8.002	-0.872	56.902		21.49	В
^^	MOTA	2378	CA	SER	331	2	9.200	-1.602	56.574	1.00	21.39	. В
30	MOTA	2379	CB	SER	331	2	9.469	-1.473	55.084	1.00	22.34	В
	ATOM	2380	OG	SER	331		0.537	-2.313	54.694		26.49	В
	MOTA	2381	C	SER	331		0.340	-1.001	57.391		20.49	В
	MOTA	2382	0	SER	331	. 3	0.418	0.208	57.565	1.00	21.48	В
	MOTA	2383	N	ILE	332	3	1.213	-1.849	57.911	1.00	18.89	В
35 ·	ATOM	2384	CA	ILE	332		2.341	-1.371	58.695		15.95	В
	ATOM	2385										
•			CB	ILE	332		2.321	-1.936	60.135		15.17	В
	ATOM	2386	CG2	ILE	332	3	3.621	-1.568	60.854	1.00	12.52	В
	MOTA	2387	CG1	ILE	332	3	1.091	-1.447	60.882	1.00	11.58	В
	MOTA	2388		ILE	332		0.932	-2.097	62.247	1.00	7.00	В
40	MOTA	2389										
TU			C	ILE	332		3.650	-1.818	58.063		15.41	В
	ATOM	2390	0	ILE	332		3.802	-2.980	57.687	1.00	12.48	В
	MOTA	2391	N	ILE	333	3	4.591	-0.888	57.948	1.00	16.21	B
	ATOM	2392	CA	ILE	333		5.899	-1.203	57.411		16.71	В
	ATOM	2393	CB	ILE	333		6.310	-0.266	56.273			
45					-						16.82	В
43	MOTA	2394	CG2	ILE	333	3	7.616	-0.744	55.675	1.00	15.94	В
	ATOM.	2395	CG1	ILE	333	3	5.242	-0.259	55.169	1.00	16.68	В
	ATOM	2396	CD1	ILE	333	3	5.557	0.705	54.012		15.18	В
	ATOM	2397	C	ILE	333		6.860	-1.021	58.561		18.56	В
50	ATOM	2398	0	ILE	333		7.074	0.104	59.032		21.41	В
50	ATOM	2399	N	ALA	334	3	7.411	-2.137	59.035	1.00	20.14	В
	ATOM	2400	CA	ALA	334	3	8.360	~2.125	60.147	1.00	19.94	В
	ATOM	2401	CB	ALA	334	3	8.182	-3.362	61.020		18.30	В
	ATOM	2402	c	ALA	334		9.756	-2.096	59.550			
											20.34	В
E E	MOTA	2403	0	ALA	334		0.135	-2.989	58.790	1.00	20.44	В
55	MOTA	2404	N	THR	335	4	0.514	-1.062	59.897	1.00	19.08	В
	ATOM	2405	CA	THR	335	4	1.853	-0.901	59.3 69	1.00	19.70	В
	MOTA	2406	CB	THR	335		2.106	0.584	59.008		21.15	В
		2407										
	MOTA			THR	335		1.876	1.409	60.157		24.31	В.
	ATOM	2408	CG2	THR	335	4	1.158	1.026	57.905	1.00	21.90	В
60	MOTA	2409	С	THR	335	4	2.907	-1.403	60.351	1.00	19.67	В
	ATOM	2410	0	THR	335		2.796	-1.190	61.559		20.81	В
	MOTA	2411	N	ILE.	336		3.924	-2.085	59.833		19.06	В
	ATOM	2412	CA	ILE	336	4	4.991	-2.618	60.680	1.00	19.16	В
	MOTA	2413	CB	ILE	336	4	4.845	-4.147	60.882	1.00	18.20	В
65	ATOM	2414		ILE	336		3.519	-4.470	61.562		17.20	В
	MOTA	2415		ILE	336		4.933	-4.857	59.564		15.56	В
	MOTA	2416	CD1	ILE	336		4.926	-6.371	59.697	1.00	16.09	В
	MOTA	2417	С	ILE	336	4	6.388	-2.343	60.116	1.00	19.85	В
	MOTA	2418	ō	ILE	336		6.547	-1.995	58.945		20.63	В
70												
, 0	ATOM	2419	N	SER	337		7.395	-2.487	60.970		21.82	В
	MOTA	2420	CA	SER	337	4	8.788	-2.277	60.576	1.00	23.86	В
	ATOM	2421	CB	SER	337	4	9.514	-1.430	61.611	1.00	22.35	В
	MOTA	2422	OG	SER	337		0.551	-2.165	62.229		19.41	В
						-			Ja. 22.	4.00	41	5

	MOTA	2423	C	SER	337	49.507	-3.622	60.458	1.00 26.10	В
	ATOM	2424	ŏ	SER	337	49.133	-4.597	61.119	1.00 25.43	В
	ATOM	2425	N	PRO	338	50.543	-3.692	59.606	1.00 26.45	В
	MOTA	2426	CD	PRO	338	50.873	-2.755	58.518	1.00 26.43	
5	MOTA	2427	CA	PRO	338		-4.943			В
J						51.287		59.441	1.00 27.75	В
	ATOM .	2428	CB	PRO	338	51.703	-4.893	58.009	1.00 25.91	В
	ATOM	2429	CC	PRO	338	52.043	-3.453	57.835	1.00 26.04	В
	ATOM	2430	C	PRO	338	52.493	-5.016	60.366	1.00 28.99	В
10	MOTA	2431	0	PRO	338	53.304	-5.929	60.250	1.00 30.27	В
10	MOTA	2432	N	ALA	339	52.615	-4.057	61.280	1.00 29.91	В
	MOTA	2433	CA	ALA	339	53.765	-4.024	62.184	1.00 31.92	В
	MOTA	2434	CB	ALA	339	54.076	-2.582	62.598	1.00 32.09	В
	MOTA	2435	С	ALA	339	53.576	-4.884	63.415	1.00 31.91	В
	ATOM	2436	0	ALA	339	52.483	-4.965	63.959	1.00 34.29	В
15	MOTA	2437	N	SER	340	54.651	-5.525	63.856	1.00 31.24	В
	MOTA	2438	CA	SER	340	54.580	-6.374	65.030	1.00 29.08	В
	MOTA	2439	СВ	SER	340	55.877	-7.280	65.138	1.00 29.57	· B
	ATOM	2440	ŌĞ	SER	340	57.053	-6.513	65.327	1.00 28.10	В
	MOTA	2441	č	SER	340	54.396	-5.555	66.307	1.00 28.00	В
20	ATOM	2442	ŏ	SER	340					
20	ATOM	2443		LEU		53.844	-6.046	67.280	1.00 28.20	В
			N		341	54.852	-4.308	66.309	1.00 28.24	В
	MOTA	2444	CA	LEU	341	54.715	-3.471	67.493	1.00 28.05	В
	ATOM	2445	CB	LEU	341	55.742	-2.306	67.463	1.00 29.43	В
25	ATOM	2446	CG	LEU	341	55.315	-0.861	67.190	1.00 30.31	В
23	MOTA	2447		LEU	341	56.404	0.084	67.690	1.00 28.26	В
	MOTA	2448		LEU	341	55.065	-0.659	65.707	1.00 31.94	В
	MOTA	2449	С	LEU	341	53.290	-2.936	67.647	1.00 28.81	В
	MOTA	2450	0	LEU	341	52.954	-2.305	68.650	1.00 28.00	В
	MOTA	2451	N	ASN	342	52.450	-3.209	66.656	1.00 28.88	В
30	MOTA	2452	CA	ASN	342	51.060	-2.780	66.690	1.00 29.97	В
	ATOM	2453	CB	ASN	342	50.689	-2.094	65.369	1.00 28.90	В
	MOTA	2454	CG	ASN	342	51.256	-0.680	65.258	1.00 29.29	В
	ATOM	2455		ASN	342	51.568	-0.210	64.161	1.00 27.68	B
	ATOM	2456		ASN	342	51.373	0.007	66.394	1.00 26.96	В
35	MOTA	2457	C	ASN	342	50.185	-4.010	66.902	1.00 31.53	В.
-	MOTA	2458	ō	ASN	342	48.958	-3.956	66.765	1.00 32.86	
	MOTA	2459	N	LEU	343					В
						50.830	-5.118	67.252	1.00 30.95	В
	MOTA	2460	CA	LEU	343	50.143	-6.387	67.474	1.00 30.40	В
40	ATOM	2461	CB	LEU	343	51.167	-7.448	67.961	1.00 31.48	В
40	MOTA	2462	CG	LEU	343	50.755	-8.930	68.109	1.00 33.60	В
	MOTA	2463		LEU	343	50.408	-9.217	69.553	1.00 34.09	В
	MOTA	2464		LEU	343	49.599	-9.270	67.168	1.00 31.95	В
	MOTA	2465	Ç	LEU	343	48.945	-6.325	68.422	1.00 28.19	В
	MOTA	2466	0	LEU	343	47.839	-6.698	68.042	1.00 29.33	` B
45	MOTA	2467	N	GLU	344	49.145	-5.858	69.647	1.00 26.96	В
	MOTA	2468	CA	GLU	344	48.035	-5.787	70.598	1.00 25.82	В
	MOTA	2469	CB	GLU	344	48.537	-5.276	71.962	1.00 27.56	В
	ATOM	2470	CG	GLU	344	47.438	-4.776	72.879	1.00 33.02	В
	MOTA	2471	CD	GLU	344	47.884	-4.708	74.329	1.00 36.74	В
50	ATOM	2472		GLU	344	49.011	-4.222	74.583	1.00 36.88	В
	MOTA	2473	OE2		344	47.104	-5.138	75.217	1.00 38.52	В
	ATOM	2474	c	GLU	344	46.843	-4.948	70.122	1.00 23.12	В
	MOTA	2475	ŏ	GLU	344	45.696	-5.357	70.265	1.00 22.53	В
	MOTA	2476	N	GLU	345	47.102	-3.775	69.564	1.00 22.13	В
55	ATOM	2477	CA	GLU	345	46.007	-2.949	69.082	1.00 22.15	
55	MOTA	2478	CB	GLU			-1.487			В
						46.484		68.830	1.00 23.16	В
	MOTA	2479	CG	GLU	345	46.722			1.00 23.64	В
	MOTA	2480	CD	GLU	345	45.440	-0.386	70.872	1.00 25.85	В
60	MOTA	2481		GLU	345	45.530	0.135	72.003	1.00 29.18	В
60	MOTA	2482		GLU	345	44.342	-0.653	70.352	1.00 25.14	В
	MOTA	2483	С	GLU	345	45.422	-3.566	67.808	1.00 21.03	В
	ATOM	2484	0	GLU	345	44.238	-3.398	67.519	1.00 20.99	В
	MOTA	2485	N	THR	346	46.253	-4.274	67.048	1.00 20.57	В
	MOTA	2486	CA	THR	346	45.794	-4.959	65.838	1.00 20.75	В
65	MOTA	2487	CB	THR	346	46.978	-5.579	65.057	1.00 21.69	В
	MOTA	2488		THR	346	47.743	-4.531	64.460	1.00 23.54	В
	MOTA	2489		THR	346	46.486	-6.540	63.964	1.00 20.78	В
	ATOM	2490	c	THR	346	44.825	-6.070	66.269	1.00 20.06	В
	MOTA	2491	ŏ	THR	346	43.824	-6.323	65.603	1.00 20.00	
70	MOTA	2492	N	LEU	347	45.127	-6.717	67.395	1.00 19.82	В
. •	ATOM	2493	CA	LEU	347	44.265		67.924		В
	ATOM	2494	CB	LEU			-7.771		1.00 20.23	В
					347	44.967	-8.547	69.080	1.00 20.75	В
	MOTA	2495	CG	LEU	347	46.123	-9.517	68.681	1.00 20.74	В

	MOTA	2496	CD1	LEU	347	46.659	-10.198	69.923	1.00 18.01	В
	ATOM	2497	CD2	LEU	347	45.630	-10.563	67.681	1.00 19.87	В
	ATOM	2498	C	LEU	347	42.950	-7.187	68.426	1.00 20.24	В
_	ATOM	2499	0	LEU	347	41.884	-7.735	68.165	1.00 20.79	В
5	MOTA	2500	N	SER	348	43.019	-6.074	69.148	1.00 19.68	. в
	MOTA	2501	CA	SER	348	41.800	-5.450	69.645	1.00 18.65	В
	MOTA	2502	CB	SER	348	42.123	-4.205	70.337	1.00 18.12	В
	ATOM	2503	OG	SER	348	42.924	-4.491	71.458	1.00 23.16	В
	MOTA	2504	С	SER	348	40.848	-5.161	68.498	1.00 18.64	В
10	MOTA	2505	0	SER	348	39.662	-5.505	68.560	1.00 17.43	В
	MOTA	2506	N	THR	349	41.377	-4.535	67.447	1.00 18.49	В
	MOTA	2507	CA	THR	349	40.577	-4.195	66.274	1.00 20.04	В
	MOTA	2508	CB	THR	349	41.440	-3.523	65.189	1.00 21.24	В
. ~	MOTA	2509	OG1	THR	349	41.774	-2.195	65.607	1.00 22.77	В
15	MOTA	2510	CG2	THR	349	40.692	-3.471	63.848	1.00 20.74	В
	MOTA	2511	С	THR	349	39.873	-5.402	65.658	1.00 20.94	В
	MOTA	2512	0	THR	349	38.651	-5.399	65.516	1.00 19.02	В
	MOTA	2513	N	LEU	350	40.645	-6.423	65.280	1.00 23.75	В
20	MOTA	2514	CA	LEU	350	40.072	-7.632	64.682	1.00 25.37	В
20	MOTA	2515	CB	LEU	350	41.155	-8.728	64.483	1.00 24.15	. В
	MOTA	2516	CG	LEU	350	42.104	-8.768	63.261	1.00 23.69	В
	ATOM	2517		LEU	350	41.548	-7.931	62.146	1.00 24.69	В.
	MOTA	2518		LEU	350	43.476	-8.294	63.652	1.00 25.26	В
25	MOTA	2519	C	LEU	350	38.967	-8.204	65.570	1.00 25.64	· B
23	MOTA	2520	0	LEU	350	37.925	-8.651	65.088	1.00 25.79	В
	MOTA	2521	N	GLU	351	39.215	-8.179	66.873	1.00 26.21	В
	MOTA	2522	CA	GLU	351	38.280	-8.705	67.859	1.00 26.22	В
	MOTA	2523	CB	GLU	351	. 38.950	-8.729	69.230	1.00 29.30	В
30	MOTA	2524 2525	CG	GLU	351	38.325	-9.722	70.181	1.00 35.95	• В
50	MOTA MOTA	2525	CD	GLU GLU	351 351	38.148	-11.081	69.528	1.00 39.86	В
	MOTA	2527		GLU	351	39.180 36.973	-11.726 -11.484	69.204	1.00 39.55	В
	MOTA	2528	,C	GLU	351	36.995	-7.887	69.326 67.927	1.00 40.87	В
	MOTA	2529	ō	GLU	351	35.886	-8.438	67.987	1.00 24.59 1.00 24.44	B B
35 [.]	ATOM	2530	N	TYR	352	37.163	-6.569	67.922	1.00 22.44	В
-	ATOM	2531	CA	TYR	352	36.058	-5.627	67.973	1.00 20.05	В
	ATOM	2532	CB	TYR	352	36.638	-4.176	68.166	1.00 20.78	В
	MOTA	2533	CG	TYR	352	35.618	-3.065	68.285	1.00 19.34	В
	ATOM	2534		TYR	352	34.997	-2.539	67.153	1.00 17.81	В
40	MOTA	2535		TYR	352	34.062	-1.515	67.258	1.00 19.71	В
	MOTA	2536		TYR	352	35.277	-2.535	69.533	1.00 19.30	В
	MOTA	2537		TYR	352	34.339	-1.507	69.649	1.00 17.88	В
	ATOM	2538	CZ	TYR	352	33.737	-1.003	68.508	1.00 19.50	В
	MOTA	2539	ОН	TYR	352	32.810	0.017	68.602	1.00 23.10	В
45	MOTA	2540	С	TYR	352	35.211	-5.723	66.706	1.00 20.25	В
	MOTA	2541	0	TYR	352	33.989	-5.704	66.776	1.00 20.39	В
	ATOM	2542	N.	ALA	353 .	35.855	-5.851	65.549	1.00 20.55	В
	MOTA	2543	CA	ALA .	353	35.122	-5.941	64.289	1.00 23.02	В
	MOTA	2544	CB	ALA	353	36.076	-5.711	63.116	1.00 20.71	В
50	MOTA	- 2545	С	ALA	353	34.374	-7.271	64.109	1.00 25.05	В
	MOTA	2546	0	ALA	353	33.259	-7.299	63.580	1.00 24.67	В
	MOTA	2547	N	HIS	354	34.983	-8.366	64.553	1.00 26.56	В
	MOTA	2548	CA	HIS	354	34.372	-9.682	64.420	1.00 29.08	В
55	MOTA	2549	CB	HIS	354	35.332	-10.761	64.917	1.00 30.47	В
23	MOTA	2550	CG	HIS	354	34.916	-12.150	64.547	1.00 31.52	В
	MOTA	2551	CD2		354		-13.156	65.293	1.00 30.23	В
	ATOM	2552	ND1		354			63.255	1.00 32.72	В
	MOTA	2553	CE1		354		-13.870	63.222	1.00 32.65	В.
60	ATOM	2554	NE2		354		-14.213	64.445	1.00 32.59	В
UU	MOTA	2555	C	HIS	354	33.059	-9.754	65.194	1.00 30.20	В
	MOTA	2556	0	HIS	354	32.075	-10.332	64.722	1.00 30.57	В
	MOTA MOTA	2557 2558	N	ARG	355	33.044	-9.177	66.390	1.00 31.47	В
	ATOM	2559	CA	ARG ARG	355 355	31.825	-9.166	67.182	1.00 33.23	В
65			CB			32.064 32.853	-8.504	68.551	1.00 35.96	В
J	MOTA MOTA	2560 2561	CG CD	ARG ARG	355 355	32.853	-9.364 -9.625	69.516	1.00 40.08	В
	MOTA	2562	NE	ARG	355 355	32.052	-8.625 -8.198	70.797 71.579	1.00 43.24 1.00 47.90	В
	ATOM	2563	CZ	ARG	355	31.127	-9.016	72.081	1.00 47.90	В
	MOTA	2564	NH1		355	31.127	-10.329	71.881	1.00 50.90	B B
70	ATOM	2565	NH2		355	30.128	-8.521	72.806	1.00 50.14	В
	MOTA	2566	C	ARG	355	30.770	-8.378	66.413	1.00 30.14	· B
	ATOM	2567	ŏ.	ARG	355	29.619	-8.801	66.321	1.00 32.82	В
	MOTA	2568	N	ALA	356	31.178	-7.240	65.850	1.00 29.87	В

	ATOM	2569	CA	ALA	356	30.266	-6.389	65.096	1.00 27.94	В
	MOTA	2570	CB	ALA	356	31.025	-5.243	64.467	1.00 28.16	В
	MOTA	2571	С	ALA	356	29.485	-7.137	64.022	1.00 26.92	В
_	MOTA	2572	0	ALA	356	28.356	-6.759	63.698	1.00 24.79	В
5	ATOM	2573	N	LYS	357	30.074	-8.203	63.486	1.00 25.84	В
•	MOTA	2574	CA	LYS	357	29.416	-8.982	62.438	1.00 27.17	В
	ATOM	2575	CB	LYS	357		-10.193	62.040	1.00 26.83	В
	ATOM	2576	CG	LYS	357	31.690	-9.905	61.724	1.00 28.45	В
	ATOM	2577	CD	LYS	357		-10.857	60.651	1.00 31.56	В
10	ATOM	2578	CE	LYS	357		-12.305	61.008		
10	MOTA	2579	NZ	LYS					1.00 31.36	
					357		-13.190	59.908	1.00 30.37	В
	MOTA	2580	C	LYS	357	28.036	-9.483	62.831	1.00 27.51	В
	ATOM	2581	0	LYS	357	27.173		61.974	1.00 27.57	В
15	ATOM	2582	N	ASN	358	27.829	-9.728	64.121	1.00 28.92	В
IJ	ATOM	2583	CA	ASN	358		-10.234	64.597	1.00 30.60	В
	ATOM	2584	CB	ASN	358		-11.024	65.911	1.00 31.34	В
	MOTA	2585	CG	ASN	358		-12.311	65.709	1.00 33.50	В
	MOTA	2586		ASN	358		-12.292	65.537	1.00 34.98	В
20	MOTA	2587		ASN	358		-13.439	65.716	1.00 33.36	В
20	MOTA	2588	С	ASN	358	25.426	-9.207	64.788	1.00 30.89	В
	MOTA	2589	0	ASN	358	24.367	-9.547	65.302	1.00 32.42	В
	MOTA	2590	N	ILE	359	25.642	-7.961	64.381	1.00 31.36	В
	ATOM	2591	CA	ILE	359	24.607	-6.943	64.530	1.00 31.09	В
~~	ATOM	2592	СB	ILE	359	25.185	-5.505	64.454	1.00 30.83	В
25	ATOM	2593	CG2	ILE	359	24.060	-4.493	64.496	1.00 28.14	В
	MOTA	2594	CG1	ILE	359	26.144	-5.246	65.629	1.00 29.88	. В
	MOTA	2595	CD1	ILE	359	27.028	-4.031	65.421	1.00 29.12	В
	MOTA	2596	С	ILE	359	23.583	-7.110	63.416	1.00 32.70	В
	ATOM	2597	0	ILE	359	23.938	-7.293	62.250	1.00 31.89	В
30	ATOM	2598	N	LEU	360	22.312	-7.045	63.795	1.00 34.93	В
	ATOM	2599	CA	LEU	360	21.195	-7.185	62.869	1.00 37.63	В
	ATOM	2600	CB	LEU	360	20.056	-7.993	63.544	1.00 39.00	В
	ATOM	2601	CG	LEU	360	18.581	-7.590	63.189	1.00 41.16	B
	MOTA	2602		LEU	360	18.283	-7.917	61.728	1.00 42.20	В
35	ATOM	2603		LEU	360	17.599	-8.315	64.118	1.00 41.50	В.
	ATOM	2604	c	LEU	360	20.672	-5.814	62.475	1.00 38.26	В
	ATOM	2605	ō	LEU	360	20.356	-5.003	63.343	1.00 38.46	В
	ATOM	2606	N	ASN	361	20.580	-5.565	61.171	1.00 39.80	В
	MOTA	2607	CA	ASN	361	20.079	-4.295	60.656		В
40	MOTA	2608	CB	ASN	361	21.133	-3.606	59.822	1.00 41.76 1.00 42.66	
	ATOM	2609	CG	ASN	361	22.088	-2.772	60.657		В
	MOTA	2610		ASN	361				1.00 44.51	В
	ATOM	2611	ND2			22.791	-3.289	61.528	1.00 45.27	В
	ATOM	2612		ASN	361	22.117	-1.467	60.394	1.00 45.23	В
45	ATOM	2613	C		361	18.825	-4.481	59.812	1.00 44.12	'B
73			0	ASN	361	18.478	-5.604	59.438	1.00 45.59	В
	MOTA	2614	N	LYS	362	18.160	-3.366	59.514	1.00 45.40	В
	MOTA	2615	CA	LYS	362	16.931	-3.332	58.716	1.00 45.80	В
	MOTA	2616	CB	LYS	362	17.226	-3.756	57.260	1.00 45.62	В
50	MOTA	2617	CG	LYS	362	17.222	-2.619	56.240	1.00 45.92	В
50	ATOM	2618	CD	LYS	362	15.832	-2.001	56.093	1.00 45.58	В
	MOTA	2619	CE	LYS	362	15.739	-1.104	54.862	1.00 43.34	В
	ATOM	2620	NZ	LYS	362	14.456	-0.345	54.818	1.00 42.49	В
	MOTA	- 2621	C	LYS	362	15.823	-4.213	59.292	1.00 47.03	В
55	MOTA	2622	0	LYS	362	15.150	-4.897	58.492	1.00 48.78	В
ככ	MOTA	2623	OXT		362	15.624	-4.198	60.526	1.00 47.26	В
	MOTA	2624	MG		2602	43.330	10.372	60.103	1.00 26.54	
	MOTA	2625	PB	ADP	2600	44.452	7.135		1.00 17.43	ADP
	MOTA	2626	01B		2600	44.951	7.845	61.612	1.00 18.86	ADP
~	MOTA	2627	02B	ADP	2600	44.008	5.637	60.747	1.00 22.98	ADP
60	ATOM	2628	03B	ADP	2600	43.299	7.848	59.790	1.00 19.76	ADP
	ATOM	2629	PA	ADP	2600	45.880	7.608	57.967	1.00 24.97	ADP
	ATOM	2630	Ola	ADP	2600	44.906	7.153	56.989	1.00 27.54	ADP
	MOTA	2631	02A	ADP	2600	45.805	9.067	58.061	1.00 29.40	ADP
/-	MOTA	2632	03A	ADP	2600	45.606	6.967	59.369	1.00 22.28	ADP
65	MOTA	2633	05*	ADP	2600	47.347	7.314	57.518	1.00 28.31	ADP
	MOTA	2634	C5*		2600	48.422	6.620	58.144	1.00 30.71	ADP
	MOTA	2635	C4*		2600	49.601	6.747	57.103	1.00 33.98	ADP
	ATOM	2636	04*		2600	49.664	5.485	56.457	1.00 33.98	ADP
	ATOM	2637	C3*		2600	49.383	7.792	55.972	1.00 32.52	ADP
70	MOTA	2638	03+		2600	50.518	8.657	55.838	1.00 36.94	ADP
	ATOM	2639	C2*		2600	49.106	7.017	54.682	1.00 35.49	ADP
	ATOM	2640	02*		2600	49.782	7.556	53.522	1.00 38.23	ADP
	ATOM	2641	C1*		2600	49.483	5.577	55.026	1.00 35.23	ADP
					2000	49.403	3.311	33.020	1.00 33.20	ADF

	MOTA	2642	N9	ADP	2600	48.437	4.548	54.689	1.00 33.78	ADP
	ATOM	2643	C8	ADP	2600	47.512	4.099		1.00 34.18	ADP
	MOTA	2644	N7	ADP	2600	46.745	3.202		1.00 36.36	ADP
_	MOTA	2645	C5	ADP	2600	47.137	3.045	53.768	1.00 36.94	ADP
5	MOTA	2646	C6	ADP	2600	46.721	2.241	52.700	1.00 37.31	ADP
	ATOM	2647	N6	ADP	2600	45.687	1.403	52.874	1.00 37.72	ADP
	MOTA	2648	Nl	ADP	2600	47.381	2.320	51.471	1.00 37.39	ADP
	ATOM	2649	C2	ADP	2600	48.446	3.171	51.268	1.00 37.76	ADP
				ADP						
10	ATOM	2650	м3		2600	48.859	.3.957	52.311	1.00 35.88	ADP
10	MOTA	2651	C4	ADP	2600	48.245	3.925	53.548	1.00 35.51	ADP
	MOTA	2652	C1	1-7	1	37.929	17.272	54.077	1.00 38.43	1-7
	MOTA	2653	C2	1-7	1	38.932	17.045	53.074	1.00 38.52	1-7
	ATOM	2654	C3	1-7	1	38.735	15.932	52.163	1.00 39.96	1-7
•	ATOM	2655	C4	1-7	ī	37.528	15.091	52.280	1.00 39.17	1-7
15	ATOM	2656	C5	1-7	ī	36.503	15.314	53.268	1.00 37.92	1-7
13										
	MOTA	2657	C6	1-7	1	36.737	16.421	54.166	1.00 39.95	1-7
	MOTA	2658		1-7	1	39.781	15.680	51.154	1.00 38.83	1-7
	MOTA	2659	N12	1-7	1	40.860	16.465	50.816	1.00 41.41	1-7
	MOTA	2660	N13	1-7	1 .	41.632	15.978	49.912	1.00 42.37	1-7
20	MOTA	2661	C14	1-7	1	41.128	14.690	49.355	1.00 40.44	1-7
	ATOM	2662		1-7	ī	40.183	14.416	50.455	1.00 39.39	1-7
	ATOM	2663		1-7	ī	41.056	14.226	47.951	1.00 36.95	1-7
	ATOM	2664		1-7	1	42.809	16.554	49.520	1.00 43.23	1-7
25	MOTA	2665		1-7	1	43.706	15.596	48.761	1.00 42.51	1-7
25	MOTA	2666	025	1-7	1	43.145	17.720	49.767	1.00 44.94	1-7
	ATOM	2667	C26	1-7	1	40.067	14.828	47.075	1.00 35.46	1-7
	MOTA	2668	C27	1-7	1	40.008	14.513	45.661	1.00 35.09	1-7
	MOTA	2669		1-7	1	40.989	13.573	45.157	1.00 34.04	1-7
	MOTA	2670		1-7	ī	41.984	12.977	46.048	1.00 34.13	1-7
30										
50	ATOM	2671		1-7	1	42.012	13.263	47.467	1.00 34.81	1-7
	MOTA		CL35		1.	37.356	13.776	51.201	1.00 40.06	1-7
	MOTA	2673	036	1-7	1	42.983	12.166	45.535	1.00 32.08	1-7
	ATOM	2674	.0	нон	2	38.525	10.810	62.766	1.00 2.98	S
	MOTA	2675	0	нон	3	23.222	11.589	60.100	1.00 22.29	S
35 ⁻	ATOM	. 2676	ŏ	нон	4	41.960	12.208	60.870	1.00 9.69	S
55	ATOM	2677	ŏ	нон	5	50.029	-4.994		1.00 18.21	
•								63.682		S
	ATOM	2678	0	нон	8	28.413	21.060	56.800	1.00 20.56	S
	MOTA	2679	0	нон	, 9	31.397		80.114	1.00 18.48	s
40	ATOM	2680	0	нон	10	38.337	3.375	65.490	1.00 21.12	S
40	ATOM	2681	0	HOH	13	45.628	22.010	69.140	1.00 9.64	s
	ATOM	2682	0	нон	14	48.257	14.330	41.733	1.00 18.62	s
	MOTA	2683	ō	НОН	15	41.014	5.558	71.890	1.00 28.07	s
	ATOM	2684	ŏ	нон	16	27.936				
							20.868	70.581	1.00 22.56	s
45	MOTA	2685	0	нон	17	43.663	-1.056	64.226	1.00 13.66	S
43	MOTA	2686	0	нон	18	43.194	8.354	64.240	1.00 19.73	s
	MOTA	2687	0	HOH	20	54.924	6.098	49.933	1.00 32.18	S
	MOTA	2688	Ο.	HOH	22	31.350	4.322	82.668	1.00 37.14	S
	ATOM	2689	0	HOH	27	45.521	-1.603	51.520	1.00 20.22	S
	ATOM	2690	ō.	HOH	28	53.208	11.559	41.772	1.00 42.11	š
50	MOTA	2691	ŏ	нон	31	27.994	6.504	79.871	1.00 18.94	S
50		2692								
	MOTA		0	НОН	33	49.291	-7.879	50.486	1.00 35.78	S
	MOTA	2693	0	нон	34	18.468	12.203	33.372	1.00 19.62	S
	ATOM	2694	0	HOH	35	53.496	-17.951	61.642	1.00 35.98	S
	ATOM	2695	0	HOH	36	45.680	3.185	45.465	1.00 19.30	S
55	MOTA	2696	0	нон	38	42.176	-0.846	72.113	1.00 14.70	S
	ATOM	2697	ō	НОН	39	51.304	5.232	60.441	1.00 24.96	Š
	ATOM	2698	ŏ	нон	40	34.806				S
			-			5			1.00 32.37	_
	MOTA	2699	0	HOH	41	19.156	14.294	56.441	1.00 28.63	S .
C O	MOTA	2700	0	нон	46	44.126	0.351	55.876	1.00 28.55	S
60 ·	MOTA	2701	0	нон	47	20.432	7.836	62.530	1.00 16.12	S
	MOTA	2702	0	нон	48	31.643	24.934	63.575	1.00 31.65	S
	ATOM	2703	0	нон	50	45.290	17.359	64.325	1.00 15.86	S
	MOTA	2704	ŏ	нон	53	41.790	5.942	40.546	1.00 28.37	S
65	ATOM	2705	0	нон	54	38.452	4.419	47.214	1.00 14.56	S
O)	MOTA	2706	0	HOH	55	52.009	4.613	57.096	1.00 35.87	S
	MOTA	2707	0	HOH	57	51.429	6.864	39.244	1.00 27.91	s
	ATOM	2708	0	HOH	58	22.685	19.136	43.047	1.00 29.36	s
	ATOM	2709	0	HOH	61	39.044	12.519	58.483	1.00 28.94	S
	ATOM	2710	ō	нон	67	45.314	-7.264	72.406	1.00 17.23	Ş
70	ATOM	2711	ŏ	нон	69	46.768	-2.040	64.134	1.00 23.58	5
. •										
	MOTA	2712	0	нон	71	45.298	18.821	48.751	1.00 30.98	S
	ATOM	2713	Ο.	HOH	79	45.903	11.457	63.308	1.00 21.87	s
	MOTA	2714	0	HOH	83	29.506	-5.557	49.394	1.00 32.50	S

	MOTA	2715	0	нон	86	28.178	4.602	77.098	1.00 29.04	s
	MOTA	2716	0	нон	89	55.210	-16.662	58.167	1.00 35.61	S
	MOTA	2717	0	нон	91	37.135	0.846	70.878	1.00 20.52	S
_	MOTA	2718	0	нон	93	17.438	19.816	52.756	1.00 35.47	S
5 -	MOTA	2719	0	HOH	94	29.881	3.798	41.417	1.00 42.97	S
	MOTA	2720	0	нон	98	39.190	3.892	49.946	1.00 13.01	Š
	ATOM	2721	0	HOH	100	41.671	15.312	56.323	1.00 31.21	S
	MOTA	2722	0	HOH	101	52.876	0.835	68.812	1.00 32.79	Š
	MOTA	2723	0	HOH	105	37.722	2.513	73.490	1.00 36.02	S
10	MOTA	2724	0	нон	109	27.450	25.927	61.040	1.00 42.15	S
	MOTA	2725	0	HOH	111	39.804	17.000	76.527	1.00 40.03	· s
	MOTA	2726	0	нон	117	2.532	6.263	36.270	1.00 22.77	Š
	MOTA	2727	0	нон	119	43.756	2.932	43.574	1.00 30.63	Š
	MOTA	2728	0	нон	124	41.324	9.248	61.513	1.00 50.60	Š
15	MOTA	2729	0	нон	128	45.349	21.055	46.092	1.00 34.28	Š
	MOTA	2730	0	нон	129	47.480	9.402	61.725	1.00 20.53	S
	ATOM	2731	0	нон	130	27.022	14.663	58.188	1.00 21.56	· s
•	MOTA	2732	0	нон	131	38.009	11.637	34.970	1.00 36.04	S
	MOTA	2733	0	нон	135	21.462	18.078	39.253	1.00 49.42	S
20	MOTA	2734	0	нон	136	50.206	-0.381	68.977	1.00 28.73	S
	ATOM	2735	0	нон	142	. 43.209	19.312	57.176	1.00 32.90	Š
	ATOM	2736	0	нон	144	27.420	-13.840	56.585	1.00 40.61	S
	MOTA	2737	0	нон	145	56.085	3.298	61.538	1.00 27.46	S
	ATOM	2738	0	HOH	148	45.044	22.181	54.899	1.00 33.67	S
25	ATOM	2739	0	нон	149	47.168	9.785	68.295	1.00 32.20	S
	ATOM	2740	0	нон	150	35.221	13.107	56.556	1.00 39.71	S
	MOTA	2741	0	. нон	156	19.494	13.147	35.697	1.00 37.79	S
	MOTA	2742	0	нон	158	35.348	1.853	79.606	1.00 35.97	S
••	MOTA	2743	0	нон	160	44.086	-3.335	73.582	1.00 28.68	S
30	MOTA	2744	0	нон	163	22.716	28.692	55.723	1.00 38.12	S
	ATOM	2745	0	нон	164	29.077	26.837	62.948	1.00 37.04	Š
	END									_

TABLE 3

	REMARK	(refi	neme	nt re	solutio	on: 50.0 - 2	2.5 A						
_	REMARK					ree_r= 0.300							
5 .						rmsd angle		268					
	REMARK	sg= P	2(1)	2(1)2	(1) a=	68.9 b= 79	.4 c= 158	8.8 alpha	= 90.	beta=	90.	gamma≃	90.
						-7_3pb.pdb						_	
	MOTA	1	CB	LYS	17		-12.099	59.933		58.09		В	
10	MOTA	2		LYS	17		-12.631	59.411		60.84		В	
10	ATOM ATOM	3 4	CD	LYS LYS	17 17		-12.482 -13.578	57.896 57.123		62.11		B B	
	MOTA	5	NZ	LYS	17		-13.570	57.123		63.01 63.35		В	
	ATOM	6	c	LYS	17	24.262	-9.737	59.096		54.65		B	
	ATOM	7	ō	LYS	17	25.150	-9.723	58.262		53.83		B	
15	MOTA	8	N	LYS	17		-10.341	61.285		56.25		В	
	MOTA	9	CA	LYS	· 17	24.364	-10.617	60.333	1.00	55.82		В	
	MOTA	10	N	ASN	18	23.168	-8.993	58.994		53.57		B	
•	MOTA	11	CA	ASN	18	22.956	-8.115	57.857		52.96		В	
20	MOTA	12	CB	ASN	18		-7.362	58.018		55.67		В	
20	ATOM	13 14	CG	ASN	18	20.433	-8.197	57.613		58.59		В	
	MOTA MOTA	15		asn asn	18 18	20.173 19.688	-9.261 -7.717	58.187 56.621		59.98 58.01		B.	
	ATOM	16	C	ASN	18	24.093	-7.115	57.635		51.27		В	
	ATOM	17	ō	ASN	18	24.391	-6.754	56.495		52.49		В	
25	MOTA	18	N	ILE	19	24.723	-6.665	58.716		47.11		В	
	MOTA	19	CA	ILE	19	25.811	-5.698	58.613		42.06		В	
	MOTA	20	CB	ILE	19	26.192	-5.152	60.004	1.00	42.31		В	
	MOTA	21		ILE	19	26.598	-6.295	60.917		43.22		В	
30	ATOM	22		ILE	19	27.343	-4.159	59.881		41.90		В	
30	MOTA	23		ILE	19	27.762	-3.556	61.193		43.78		В	
	MOTA MOTA	24 25	0	ILE ILE	19 19	27.054 27.480	-6.300 -7.376	.57.958 58.312		38.26 38.23		B B	
	ATOM	26	N	GLN	20	27.627	-5.577	56.999		34.90		В	
	ATOM	27	CA	GLN	20	28.820	-6.021	56.279		30.15		В	
35	MOTA	28	CB	GLN	20	28.778	-5.516	54.838		27.85		В	
	MOTA	29	CG	GLN	20	30.034	-5.802	54.038	1.00	26.74		В	
	MOTA	30	CD	GLN .	20	29.987	-5.186	52.643	1.00	27.60		В	
	MOTA	31		GLN	20	30.137	-3.9B4	52.484		29.30		В	
40	MOTA	32		GLN	20	29.774	-6.017	51.632		26.15		В	
40	MOTA	33	C	GLN	20	30.091	-5.507	56.949		29.28		В	
	MOTA MOTA	34 35	O N	GLN VAL	20 21	30.186	-4.346 -6.379	57.290		29.19		B B	
	MOTA	36	CA	VAL	21	31.075 32.325	-5.975	57.127 57.754		27.08		В	
	ATOM	37	CB	VAL	21	32.448	-6.546	59.180		24.84		В	
45	ATOM	38		VAL	21	33.766	-6.123	59.804	1.00			В	
	ATOM	39		VAL	21	31.274	-6.078	60.033		24.09		В	
	MOTA	40	С	VAL .	21	33.524	-6.439	56.938	1.00	24.57		В	
	MOTA	41	0	VAL	21	33.677	-7.608	56.687		24.54		В	
50	MOTA	42	N	VAL	22	34.370	-5.496	56.531		25.16		В	
50	MOTA MOTA	43 44	CA	VAL	22	35.558	-5.818	55.753		24.51		В	
	ATOM	45	CB	VAL VAL	22 22	35.493 34.274	-5.171 -5.694	54.356 53.602		25.74		B B	
	ATOM	46		VAL	22	35.428	-3.648	54.488		26.13		В	
	ATOM	47	c	VAL	22	36.825	-5.350	56.464		24.25		В	
55	MOTA	48	0	VAL	22	36.769	-4.532	57.376		25.41		В	
	ATOM	49	N	VAL	23	37.964	-5.889	56.047		21.62		В	
	ATOM	50	CA	VAL	23	39.249	-5.541	56.640	1.00	20.21		В	
	ATOM	51	CB	VAL	23	39.875	-6.749	57.398		19.81		В	
60	ATOM	52		VAL	23	41.246						В	
60	MOTA	53		VAL	23	38.980	-7.164	58.552		19.57		В	
	MOTA MOTA	54 55	0	VAL VAL	23 23	40.224	-5.069 -5.587	55.565		20.21		В	
	MOTA	56	N	ARG	24	40.231 41.026	-4.063	54.453 55.908		18.34 20.97		B B	
	ATOM	57	CA	ARG	24	42.012	-3.508	54.987		23.76		В	
65	ATOM	58	СВ	ARG	24	41.493	-2.221	54.341		19.71		В	
	ATOM	59	CG	ARG	24	42.364	-1.729	53.201		19.19		В	
	MOTA	60	CD	ARG	24	42.064	-0.294	52.784		17.94		В	
	MOTA	61	NE	ARG	24	42.664	0.010	51.487		16.57		В	
70	MOTA	62	CZ	ARG	24	42.479	1.134	50.801		18.90		В	
70	MOTA	63		ARG	24	41.704	2.100	51.281		16.81		В	
	MOTA	64	NH2	ARG	24	43.057	1.275	49.615	1.00	16.05		В	

	ATOM	65	С	ARG	24	43.304	-3.210	55.736	1.00 27.05	В
	ATOM	66	0	ARG	24	43.313	-2.442	56.712	1.00 27.85	В
	ATOM	67	N	CYS	25	44.392	-3.820	55.274	1.00 29.51	В
	ATOM	68	CA	CYS	25	45.699	-3.637	55.890	1.00 32.32	В
5										
5	ATOM	69	CB	CYS	25	46.410	-4.991	56.027	1.00 30.86	В
	ATOM	70	SG	CYS	25	48.111	-4.890	56.627	1.00 32.54	В
	ATOM	71	С	CYS	25	46.545	-2.696	55.045	1.00 33.84	В
	MOTA	72	0	CYS	25	46.587	-2.820	53.831	1.00 35.92	В
	MOTA	73	N	ARG	26	47.218		55.694	1.00 34.94	В
10	MOTA	74	CA	ARG	26	48.053	-0.807	54.967	1.00 37.11	В
10										
	ATOM	75	CB	ARG	26	48.130	0.526	55.723	1.00 37.77	В
	ATOM	76	CG	ARG	26	48.388	0.384	57.222	1.00 37.85	В
	MOTA	77	CD	ARG	26	49.107	1.591	57,802	1.00 36.08	В
	ATOM	78	NE	ARG	26	50.554	1.433	57.704	1.00 35.38	В
15	ATOM	79	CZ	ARG	26	51.379	1.390	58.747	1.00 35.56	В
	MOTA	80		ARG	26	50.910	1.502	59.982	1.00 32.33	В
	ATOM	81	NH2	ARG	26	52.677	1.209	58.551	1.00 37.10	• в
	MOTA	82	C	ARG	26	49.463	-1.341	54.751	1.00 38.55	В
20	ATOM	83	0	ARG	26	49.917	-2.224	55.460	1.00 38.07	В
20	MOTA	84	N	PRO	27	50.170	-0.806	53.752	1.00 40.05	В
	MOTA	85	CD	PRO	27	49.674	0.092	52.693	1.00 41.26	В
	MOTA	86	CA	PRO	27	51.536	-1.244	53.467	1.00 42.07	В
	ATOM	87	СВ	PRO	27	51.734	-0.805	52.021	1.00 42.46	B
	ATOM	88	CG	PRO	27	50.945	0.468	51.961	1.00 41.54	8
25										
25	MOTA	89	C	PRO	27	52.508	-0.555	54.418	1.00 43.29	В
	ATOM	90	0	PRO	27	52.115	0.329	55.170	1.00 43.49	. В
	ATOM	91	N	PHE	28	53.773	-0.968	54.380	1.00 45.76	В
	ATOM	92	CA	PHE	28	54.807	-0.381	55.233	1.00 47.49	В
	MOTA	93	CB	PHE	28	56.045	-1.290	55.308	1.00 46.30	В
30	ATOM	94	CG	PHE	28	55.770	-2.659	55.861	1.00 45.96	В
-	MOTA	95		PHE	28		-3.709		1.00 45.49	
						55.424		55.015		В
	MOTA	96		PHE	28	55.849	-2.899	57.230	1.00 45.19	В
	MOTA	97	CE1		28.	55.162	-4.976	55.526	1.00 44.86	В
~ -	MOTA	98	CE2	PHE	28	55.588	-4.165	57.751	1.00 44.92	В
35	MOTA	99	CZ	PHE	28	55.244	-5.204	56.897	1.00 43.96	В.
	ATOM	100	С	PHE	28	55.240	0.974	54.686	1.00 49.68	В
	ATOM	101	ō	PHE	28	55.458	1.127	53.484	1.00 50.76	В
	ATOM	102	N	ASN	29	55.369	1.955	55.572	1.00 51.78	В
40	MOTA	103	CA	ASN	29	55.791	3.289	55.164	1.00 53.98	В
40	ATOM	104	CB	ASN	29	55.477	4.303	56.268	1.00 52.37	В
	ATOM	105	CG	ASN	29	55.889	3.818	57.647	1.00 51.95	В
	MOTA	106	OD1	ASN	29	57.068	3.614	57.918	1.00 51.68	В
	ATOM	107		ASN	29	54.909	3.633	58.526	1.00 50.23	В
	ATOM	108	c	ASN	29	57.285	3.275	54.841	1.00 56.89	В
45										
73	MOTA	109	0	ASN	29	57.973	2.293	55.111	1.00 57.68	В
	MOTA	110	N	LEU	30	57.779	4.361	54.257	1.00 59.05	В
	MOTA	111	CA	LEU	30	59.185	4.452	53.882	1.00 60.93	В
	MOTA	112	CB	LEU	30	59.466	5.837	53.293	1.00 60.81	В
	MOTA	113	CG	LEU	30	60.555	5.909	52.218	1.00 61.25	В
50	ATOM	114	CD1		30	60.401	7.199	51.429	1.00 61.39	В
-	ATOM	115	CD2		30	61.935	5.810	52.856	1.00 61.13	В
	MOTA	116		LEU	30			55.047		
			C			60.136	4.167		1.00 62.80	B
	MOTA	117	0	LEU	30	61.206	3.611	54.852	1.00 63.36	В
	MOTA	118	N	ALA	31	59.736	4.545	56.257	1.00 64.56	В
55	ATOM	119	CA	ALA	31	60.565	4.326	57.440	1.00 66.24	В
	MOTA	120	CB	ALA	31	59.999	5.104	58.617	1.00 64.93	В
	MOTA	121	С	ALA	31	60.671	2.846	57.798	1.00 68.38	В
	MOTA	122	ō	ALA	31	61.757	2.345	58.088	1.00 69.26	В
	MOTA	123	N	GLU	32				1.00 69.84	
60						59.537	2.153	57.781		В
UU	MOTA	124	CA	GLU	32	59.492	0.734	58.107	1.00 71.88	В
	MOTA	125	CB	GLU	32	58.038	0.275	58.225	1.00 70.67	В
	ATOM	126	CG	GLU	32	57.338	0.752	59.487	1.00 67.99	B
	ATOM	127	CD	GLU	32	55.831	0.607	59.412	1.00 65.98	В
	ATOM	128	OE1		32	55.174	0.723	60.468	1.00 65.36	. B
65	ATOM	129	OE2		32	55.302	0.383	58.301		
55									1.00 62.48	В
	MOTA	130	C	GLU	32	60.232	-0.143	57.097	1.00 74.40	В
	MOTA	131	0	GLU	32	61.090	-0.930	57.472	1.00 74.92	В
	MOTA	132	N	ARG	33	59.897	-0.008	55.816	1.00 76.35	В
	ATOM	133	CA	ARG	33	60.550	-0.803	54.779	1.00 78.32	В
70	ATOM	134	CB	ARG	33	59.936	-0.502	53.407	1.00 79.77	B
-	MOTA	135	CG	ARG	33	59.972	0.964	53.010	1.00 83.18	В
	ATOM	136	CD	ARG	33	59.329			1.00 85.46	
							1.183	51.645		В
	MOTA	137	NE	ARG	33	60.032	0.459	50.589	1.00 87.40	B

	ATOM	138	CZ	ARG	33	61.269	0.737	50.186	1 00 00 75	
•									1.00 88.75	В
	MOTA	139	NH1		33	61.948	1.729	50.747	1.00 89.79	В
	MOTA	140	NH2		33	61.828	0.019	49.221	1.00 89.07	Э
_	MOTA	141	С	ARG	33	62.053	-0.536	54.754	1.00 78.80	В
5	MOTA	142	Ō	ARG	33	62.832	-1.379	54.318	1.00 78.36	В
	ATOM	143	N	LYS	34	62.448	0.644	55.226	1.00 79.39	В
	MOTA	144	CA	LYS	34	63.853	1.029	55.284	1.00 80.19	В
	ATOM	145	_	LYS		63.984		55.504	1.00 80.19	
			CB		34		2.543			В
10	MOTA	146	CG.	LYS	34	64.392	.3.347	54.267	1.00 82.59	В
10	MOTA	147	CD	LYS	34	65.910	3.501	54.147	1.00 83.41	В
	MOTA	148	. CE	LYS	34	66.604	2.186	53.810	1.00 84.19	В
	MOTA	149	NZ	LYS	34	68.089	2.305	53.845	1.00 84.38	В
	MOTA	150	C	LYS	34	64.539	0.285	56.423	1.00 80.45	В
•	ATOM	151	ŏ	LYS	34	65.757	0.159	56.448	1.00 81.20	B
15				ALA	35		-0.209			
13	MOTA	152	N			63.740		57.365	1.00 80.19	В
	MOTA	153	CA	ALA	35	64.264	-0.946	58.509	1.00 79.99	В
	MOTA	154	CB	ALA	35	63.654	-0.405	59.800	1.00 79.19	В
	MOTA	155	С	ALA	35	63.966	-2.441	58.372	1.00 79.54	В
	MOTA	156	0	ALA	35	64.029	-3.181	59.347	1.00 79.52	В
20	MOTA	157	N	SER	36	63.650	-2.870	57.150	1.00 79.23	В
	ATOM	158	CA	SER	36	63.324	-4.269	56.866	1.00 78.90	B
	MOTA	159	СВ	SER	36	64.581	-5.140	56.934	1.00 79.55	В
	MOTA	160			36					
			OG	SER		65.497	-4.786	55.913	1.00 80.94	В
25	ATOM	161	C	SER	36	62.291	-4.773	57.863	1.00 77.94	· B
23	ATOM	162	0	SER	- 36	62.621	-5.460	58.826	1.00 78.06	В
	MOTA	163	N	ALA	37	61.033	-4.422	57.620	1.00 76.14	В
	MOTA	164	CA	ALA	37	59.952	-4.822	58.505	1.00 74.02	В
	MOTA	165	СВ	ALA	37	58, 862	-3.763	58.496	1.00 74.76	В
	ATOM	166	С	ALA	37	59.370	-6.177	58.128	1.00 72.27	. B
30	MOTA	167	ŏ	ALA	37	59.282	-6.526	56.956	1.00 71.83	В
	MOTA	168	N	HIS	38	58.975	-6.928			
								59.151	1.00 70.33	В
	MOTA	169	CA	HIS	38	58.388	-8.249	58.981	1.00 67.10	В
	ATOM	170	СВ	HIS	38	59.039	-9.236	59.961	1.00 69.95	В
25	ATOM	171	CG	HIS	38	59.177	-8.706	61.358	1.00 72.03	В
35	ATOM -	. 172	CD2	HIS	38	58.589	-9.085	62.518	1.00 72.68	В
	MOTA	173	ND1	HIS	38	60.004	-7.648	61.676	1.00 72.05	В
	MOTA	174	CE1	HIS	38	59.919	-7.399	62.971	1.00 72.38	В
	ATOM	175		HIS	38	59.067	-8.256	63.505	1.00 73.14	В
	MOTA	176	c	HIS	38					
40						56.877	-8.187	59.220	1.00 63.55	В
40	MOTA	177	0	HIS	38	56.426	-7.917	60.335	1.00 63.33	В
	MOTA	178	N	SER	39	56.100	-8.432	58.168	1.00 58.67	В
	MOTA	179	CA	SER	39	54.643	-8.399	58.266	1.00 54.45	В
	MOTA	180	CB	SER	39	54.005	-8.478	56.879	1.00 53.84	В
	MOTA	181	OG	SER	39	52.595	-8.614	56.976	1.00 49.31	В
45	MOTA	182	С	SER	39	54.081	-9.519	59.122	1.00 52.25	В
	MOTA	183	ō	SER	39		-10.686	58.910	1.00 51.84	В
	MOTA	184	N.	ILE	40	53.251	-9.149	60.089	1.00 49.22	В
	ATOM	185	CA	ILE	40					
							-10.122	60.967	1.00 47.52	В
50	MOTA	186	CB	ILE	40	52.679	-9.674	62.444	1.00 45.91	В
50	ATOM	187	CG2		40	54.115	-9.499	62.881	1.00 44.82	В
	ATOM	188	CG1		40	51.915	-8.361	62.622	1.00 45.54	В
	MOTA	1.89	CD1	ILE	40	51.580	-8.050	64.066	1.00 46.62	В
	MOTA	190	С	ILE	40	51.176	-10.316	60.557	1.00 47.28	В
	MOTA	191	0	ILE	40	50.421	-10.994	61.234	1.00 46.90	В
55	MOTA	192	N	VAL	41	50.798	-9.718	59.433	1.00 47.41	В
	ATOM	193	CA	VAL	41	49.430	-9.824	58.939	1.00 48.95	В
	MOTA							58.983		
		194	CB	VAL	41	48.713	-8.450		1.00 49.16	В
	ATOM	195	CG1		41	47.290	-8.585	58.467	1.00 49.01	В.
۲۸	MOTA	196	CG2		41	48.713	-7.903	60.402	1.00 49.06	В
60	MOTA	197	С	VAL	41		-10.347	57.509	1.00 49.67	В
	MOTA	198	0	VAL	41	50.004	-9.777	56.620	1.00 49.95	В
	MOTA	199	N	GLU	42	48.685	-11.449	57.301	1.00 50.48	В
	ATOM	200	CA	GLU	42		-12.024	55.969	1.00 51.59	В
	ATOM	201	CB	GLU	42		-13.434	55.935	1.00 52.66	В
65	ATOM	202	CG	GLU	42		-13.510	56.447	1.00 56.16	
55										В
	MOTA	203	CD	GLU	42		-14.931	56.476	1.00 58.24	В
	MOTA	204	OE1		42		-15.854	56.899	1.00 57.80	В
	MOTA	205	OE2		42		-15.119	56.081	1.00 58.28	В
70	MOTA	206	С	GLU	42		-12.072	55.599	1.00 50.83	В
70	ATOM	207	0	GLU	42	46.283	-12.604	56.343	1.00 51.55	В
	ATOM	208	N	CYS	43		-11.493	54.453	1.00 49.80	В
	ATOM	209	CA	CYS	43		-11.473	53.995	1.00 49.65	В
	MOTA	210	CB	CYS	43		-10.087	53.433	1.00 49.83	
	NI ON	210	CD	-13	4.0	40.00/	-10.00/	33.433	1.00 49.93	В

	3004	211	00	0110	4.7	45 010	0 745	E 4 CC1	3 00 40 70	_
	MOTA	211	SG	CYS	43	45.019	-8.745	54.661	1.00 48.78	В
	ATOM	212	С	CYS	43	45.140	-12.535	52.931	1.00 48.94	В
	ATOM	213	Ō	CYS	43	46.010	-12.833	52.123	1.00 48.97	В
			-		-					
	ATOM	214	N	ASP	44	43.939	-13.105	52.954	1.00 49.14	В
5				ASP						
J	MOTA	215	CA		44		-14.121	51.992	1.00 48.86	В
	MOTA	216	CB	ASP	44	43.463	-15.494	52.660	1.00 50.97	В
	MOTA	217	CG	ASP	44	43.589	-16.635	51.666	1.00 52.32	В
	ATOM	218	OD1	ASP	44	43.126	-16.483	50.510	1.00 52.22	В
4 🛕	ATOM	219	OD2	ASP	44	44.14/	-17.689	52.048	1.00 52.81	В
10	ATOM	220	С	ASP	44	42.150	-13.749	51.456	1.00 48.60	В
	MOTA	221	0	ASP	44	41.127	-14.147	52.012	1.00 46.42	В
	ATOM	222	N	PRO	45	42 108	-12.969	50.364	1.00 48.35	В
	ATOM	223	CD	PRO	45	43.252	-12.517	49.557	1.00 48.19	В
	MOTA	224	CA	PRO	45	40 847	-12.540	49.755	1.00 48.75	В
15										
13	ATOM	225	CB	PRO	45	41.307	-11.680	48.584	1.00 49.00	В
	MOTA	226	CG	PRO	45	42 617	-12.306	48.211	1.00 49.04	В
	ATOM	227	С	PRO	45	39.957	-13.688	49.312	1.00 50.08	В
	ATOM	228	0	PRO	45	38 750	-13.661	49.535	1.00 50.55	В
	ATOM	229	N	VAL	46	40.561	-14.693	48.683	1.00 50.66	В
20	ATOM	230	CA	VAL	46	39 818	-15.851	48.213	1.00 50.49	В
	MOTA	231	СB	VAL	46	40.745	-16.853	47.500	1.00 50.30	В
	MOTA	232	CG1	VAI.	46	39.957	-18.079	47.077	1.00 49.67	В
	MOTA	233	CG2	VAL	46	41.393	-16.192	46.293	1.00 49.30	В
	MOTA	234	С	VAL	46	39.145	-16.545	49.389	1.00 50.88	. В
25										
23	ATOM	235	0	VAL	46	37.965	-16.870	49.338	1.00 52.16	B
	ATOM	236	N	ARG	47	39.906	-16.761	50.454	1.00 49.91	. В
	ATOM	237	CA -	ARG	47	39.369	-17.417	51.635	1.00 49.25	В
	ATOM	238	ÇВ	ARG	47	40.499	-18.074	52.431	1.00 53.01	В
	MOTA	239	CG	ARG	47	40.025	-19.009	53.535	1.00 58.79	В
30	· ATOM	240	CD	ARG	47	30 711	-20.404	52.993	1.00 62.76	В
50										
	ATOM	241	NE	ARG	47	40.925	-21.094	52.566	1.00 65.61	В
	ATOM	242	CZ	ARG	47	41.887	-21.489	53.395	1.00 67.31	В
	ATOM	243	NH1	ARG	47	41.770	-21.265	54.699	1.00 67.77	В
	ATOM	244	NH2	ARG	47	42.970	-22.093	52.922	1.00 67.97	В
35										
22	MOTA	245	С	ARG	47	38.649	-16.396	52.518	1.00 46.27	В
	MOTA	246	0	ARG	47	37 980	-16.767	53.479	1.00 45.17	В
	MOTA	247	N	LYS	48	38.789	-15.116	52.167	1.00 43.30	В
	MOTA	248	CA	LYS	48	30 101	-14.003	52.911	1.00 40.30	В
	MOTA	249	CB	LYS	48	36.660	-14.063	52.861	1.00 40.48	В
40	MOTA	250		LYS	48	26 024	-13.999	51.466	1.00 42.10	
70										В
	MOTA	251	CD	LYS	48	34.566	-14.224	51.491	1.00 46.49	В
		252								
	MOTA			LYS	48		-14.463	50.088	1.00 48.94	В
	ATOM	253	NZ	LYS	48	34.342	-13.358	49.137	1.00 51.33	В
	ATOM	254		LYS	48		-14.040			
AF								54.364	1.00 38.40	B
45	ATOM	255	0	LYS	48	37.879	-13.780	55.271	1.00 37.06	В
				GLU	49					
	MOTA	256					-14.374	54.573	1.00 38.43	В
	MOTA	257	CA	GLU	49	40.472	-14.451	55.918	1.00 38.68	В
	MOTA	258		GLU	49		-15.867	56.237	1.00 42.04	
										В
	MOTA	259	CG	GLU	49	39.896	-16.940	56.342	1.00 47.74	В
50	MOTA	260	CD	GLU	49	40 470	-18.320	56.671	1.00 49.86	В
50										
	MOTA	261	OE1	GLU	49	39.706	-19.305	56.666	1.00 50.42	В
	MOTA	262	OE2	GLII	49	41 701	-18.419	56.930	1.00 49.85	В
	MOTA	263	С	GLU	49	41.643	-13.506	56.111	1.00 37.41	В
	ATOM	264	0	GLU	49	42.273	-13.066	55.158	1.00 34.84	В
55										
22	MOTA	265	N	VAL	50	41.925	-13.220	57.374	1.00 36.48	В
	MOTA	266	CA	VAL	50	43.035	-12.366	57.751	1.00 37.37	В
	MOTA	267	CB	VAL	50	42.539	-10.930	58.146	1.00 37.30	В
	MOTA	268	CG1	VAI.	50		-11.008	59.061	1.00 38.02	В
	MOTA	269	CG2	VAL	50	43.655	-10.153	58.813	1.00 36.20	В
60	MOTA	270		VAL	50		~13.074	58.921	1.00 36.84	В
	MOTA	271	0	VAL	50	43.078	-13.354	59.926	1.00 37.07	В
	ATOM	272		SER	51		-13.399	58.772	1.00 37.03	В
	MOTA	273	CA	SER	51	45.702	-14.095	59.835	1.00 37.03	В
	MOTA	274		SER	51		-15.390	59.294	1.00 37.38	
65										. В
65	MOTA	275	OG	SER	51	46.507	-16.327	60.339	1.00 38.42	В
	ATOM	276			51					
				SER			-13.217	60.436	1.00 37.30	В
	MOTA	277	0	SER	51	47.538	-12.567	59.712	1.00 37.32	В
	ATOM	278		VAL	52		-13.207			
								61.764	1.00 37.43	В
	ATOM	279	CA	VAL	52	47.861	-12.398	62.476	1.00 40.09	В
70										
, 0	MOTA	280		VAL	52		-11.380	63.433	1.00 38.82	В
	MOTA	281	CG1	VAL	52	48.210	-10.529	64.140	1.00 38.44	В
	MOTA	282	CG2		52		-10.507	62.664	1.00 39.75	В
	MOTA	283	С	VAL	52	48.814	-13.254	63.307	1.00 41.41	В
			-							_

	MOTA	284	0	VAL	52	48.383 -14.120 64.059 1.00 42.26	В
	MOTA	285	N	ARG	53	50.112 -13.001 63.170 1.00 42.93	В
	MOTA	286	CA	ARG	53	51.115 -13.746 63.922 1.00 44.63	В
	MOTA	287	CB	ARG	53	52.435 -13.782 63.156 1.00 44.21	В
5							
,	ATOM	288	CG	ARG	53	53.621 -14.258 63.976 1.00 45.18	В
	MOTA	289	CD	ARG	53	54.721 -14.772 63.069 1.00 47.32	В
	MOTA	290	NE	ARG	53	55.045 -13.815 62.016 1.00 48.93	В
	MOTA	291	CZ	ARG	53	55.538 -14.154 60.831 1.00 48.81	В
	MOTA	292	NH1	ARG	53	55.762 -15.430 60.548 1.00 49.29	В
10	MOTA	293	NH2	ARG	53	55.804 -13.221 59.928 1.00 50.89	В
	ATOM	294	С	ARG	53	51.333 -13.130 65.298 1.00 46.43	В
	MOTA	295	0	ARG	53	51.867 -12.030 65.420 1.00 47.02	В
	MOTA	296	N	THR	54	50.915 -13.855 66.331 1.00 48.25	В
•	ATOM	297	CA	THR	54	51.052 -13.401 67.711 1.00 50.92	
15							В
17	ATOM	298	CB	THR	54	49.768 -13.683 68.512 1.00 50.31	В
	ATOM	299	0G1	THR	54	49.572 -15.098 68.631 1.00 50.23	В
	ATOM	300	CG2	THR	54	48.567 -13.078 67.810 1.00 50.24	В
	ATOM	301	С	THR	54	52.211 -14.097 68.412 1.00 53.34	В
	ATOM	302	0	THR	54	52.551 -13.769 69.538 1.00 53.13	В
20	MOTA	303	N	GLY	55	52.815 -15.059 67.726 1.00 57.17	. В
	MOTA	304	CA	GLY	55	53.917 -15.805 68.303 1.00 61.42	В
	MOTA	305	С	GLY	55	55.300 -15.366 67.868 1.00 64.33	В
	ATOM	306	0	GLY	55	55.566 -14.175 67.715 1.00 65.05	B [']
25	MOTA	. 307	N	GLY	56	56.181 -16.346 67.672 1.00 66.22	· B
25	MOTA	308	CA	GLY	56	57.548 -16.061 67.272 1.00 68.09	В
	MOTA	309	С	GLY	56	57.760 -15.914 65.777 1.00 69.96	В
	MOTA	310		GLY	56		
			.0				В
	MOTA	311	N	LEU	57 .	58.860 -16.484 65.288 1.00 71.01	В
	MOTA	312	CA	LEU	57	59.220 -16.421 63.873 1.00 70.64	В
30	ATOM	313	CB	LEU	57	60.702 -16.771 63.704 1.00 71.42	В
50							
	MOTA	314	CG	LEU	57	61.326 -17.671 64.778 1.00 71.92	В
	ATOM	315	CD1	LEU	57	60.653 -19.034 64.777 1.00 72.30	В
•	ATOM	316	CD2		57	62.819 -17.813 64.522 1.00 72.27	В
25.	MOTA	317	С	LEU	57	58.366 -17.311 62.973 1.00 70.34	В
.35	-MOTA	. 318	0	LEU	57	57.535 -18.083 63.450 1.00 69.85	В
	ATOM	319	N	ALA	58	58.589 -17.189 61.667 1.00 69.38	В
	MOTA	320	CA	ALA	58	57.852 -17.959 60.669 1.00 68.14	В
	ATOM	321	СВ	ALA	58	58.16917.430 59.268 1.00 68.25	В
	MOTA	322	С	ALA	58	58.129 -19.462 60.742 1.00 66.52	В
40							
70	MOTA	323		·ALA	58	57.262 -20.268 60.433 1.00 66.64	В
	MOTA	324	N	ASP	59	59.343 -19.825 61.150 1.00 64.49	В
	MOTA	325	CA	ASP	59	59.743 -21.226 61.270 1.00 62.67	В
	ATOM	326	СВ	ASP	59		В
45	MOTA	327	CG	ASP	59	61.589 -22.724 62.197 1.00 61.33	В
45	MOTA	328	OD1	ASP	59	61.727 -23.594 61.307 1.00 59.84	В
	MOTA	329	OD2		59	61.772 -22.963 63.410 1.00 60.73	В
	ATOM	330	C.	ASP	59	58.801 -21.994 62.201 1.00 61.33	В
	MOTA	331	0	ASP	59	58.542 -23.182 62.005 1.00 60.81	В
	MOTA	332	N·	LYS	60	58.287 -21.302 63.211 1.00 59.03	В
50	MOTA	333	CA	LYS	60		
50						57.376 -21.897 64.179 1.00 57.28	В
	MOTA	334	CB	LYS	60	58.147 -22.816 65.134 1.00 57.38	В
	ATOM	335	CG	LYS	60	57.281 -23.524 66.164 1.00 57.92	В
	MOTA	336	CD	LYS	60	58.117 -24.299 67.172 1.00 58.61	В
	ATOM						
E E		337	CE	LYS	60	57.247 -24.930 68.245 1.00 58.86	В
55	MOTA	338	NZ	LYS	60	58.064 -25.535 69.333 1.00 59.92	В
	MOTA	339	С	LYS	60	56.710 -20.771 64.968 1.00 55.75	В
	ATOM	340			60		
			0	LYS		57.391 -19.942 65.574 1.00 55.85	В
	MOTA	341	N	SER	61	55.381 -20.735 64.953 1.00 52.88	В.
	ATOM	342	CA	SER	61	54.655 -19.692 65.666 1.00 50.87	В
60	MOTA	343					
00			CB	SER	61		В
	MOTA	344	OG	SER	61	54.294 -18.346 63.667 1.00 48.16	В
	MOTA	345	С	SER	61	53.158 -19.957 65.796 1.00 50.20	В
	ATOM	346	ō				
				SER	61		В
65	MOTA	347	N	SER	62	52.493 -19.086 66.547 1.00 49.11	В
65	ATOM	34B	CA	SER	62	51.055 -19.170 66.752 1.00 48.21	В
	MOTA	349	CB	SER	62		
							В
	MOTA	350	0G	SER	62	51.371 -17.993 68.858 1.00 48.30	В
	MOTA	351	С	SER	62	50.421 -17.990 66.010 1.00 48.13	В
	MOTA	352	ō	SER	62	51.097 -17.016 65.703 1.00 47.13	В
70							
, 0	ATOM	353	N	ARG	63	49.129 -18.085 65.712 1.00 47.13	В
	MOTA	354	CA	ARG	63	48.441 -17.015 64.998 1.00 45.05	В
	MOTA	355	CB.	ARG	63	48.539 -17.231 63.481 1.00 44.51	В
	MOTA	356	CG	ARG	63	49.960 -17.194 62.925 1.00 44.98	В

	MOTA	357	CD	ARG	63	49.976	-17.466	61.428	1.00 46.63	В
	ATOM				63					
		358	NE	ARG	-		-16.349	60.645	1.00 48.69	В
	ATOM	359	CZ	ARG	63	50.148	-15.285	60.263	1.00 48.66	В
	ATOM	360	NH1	ARG	63	51.429	-15.178	60.587	1.00 49.48	В
5	ATOM									
,		361	NH2		63		-14.329	59.545	1.00 48.53	В
	ATOM	362	С	ARG	63	46.975	-16.918	65.401	1.00 43.84	В
	ATOM	363	0	ARG	63	46.477	-17.726	66.176	1.00 44.06	В
	MOTA	364	N	LYS	64		-15.902	64.868	1.00 42.24	В
	MOTA	365	CA	LYS	64	44.892	-15.652	65.124	1.00 40.40	В
10	ATOM	366	CB	LYS	64	44 723	-14.434	66.032	1.00 41.92	В
	ATOM	367	CG	LYS	64		-14.635	67.470	1.00 43.37	В
	MOTA	368	CD	LYS	64	44.088	-15.261	68.317	1.00 43.81	В
	ATOM	369	CE	LYS	64	44.446	-15.213	69.794	1.00 45.77	В
	ATOM									
15		370	NZ	LYS	64		-15.792	70.658	1.00 46.88	В
15	MOTA	371	С	LYS	64	44.257	-15.369	63.771	1.00 39.22	В
	MOTA	372	0	LYS	64	44.631	-14.405	63.102	1.00 39.99	В
	ATOM	373	N	THR	65	43.312				
								63.361	1.00 36.46	В
	MOTA	374	CA	THR	65	42.656	-16.031	62.074	1.00 34.76	В
	ATOM	375	CB	THR	65	42.745	-17.323	61.212	1.00 35.41	В
20	MOTA	376	0G1		65	44.118		61.041		
									1.00 32.86	В
	MOTA	377	CG2	THR	65	42.130	-17.090	59.826	1.00 36.73	В
	MOTA	378	С	THR	65	41.194	-15.638	62.238	1.00 34.16	В
	MOTA	379	0	THR	65	40.477		63.070	1.00 35.43	В
25	MOTA	380	N	TYR	66	40.764		61.448	1.00 30.66	В
25	MOTA	381	CA	TYR	66	39.391	-14.181	61.488	1.00 28.38	В
	MOTA	382	СВ	TYR	66	39.337		62.072		. B
	MOTA	383	CG	TYR	66	39.886		63.473	1.00 22.38	В
	ATOM	384	CD1	TYR	66	41.255	-12.566	63.710	1.00 20.36	В
	MOTA	385	CE1	TYR	66	41.753	-12 475	65.011	1.00 19.50	В
30	ATOM	386		TYR	66	39.027				
50								64.569	1.00 22.45	В
	MOTA	387	CE2	TYR	66	39.506	-12.559	65.868	1.00 19.18	В
	MOTA	388	CZ	TYR	66	40.865	-12.470	66.086	1.00 21.06	В
	ATOM	389	ОН	TYR	66					
						41.317		67.391	1.00 25.17	В
~~	MOTA	390	С	TYR	66	38.815	-14.171	60.076	1.00 29.18	В
35	ATOM	391	0	TYR	66	39.537	-13.953	59.108	1.00 29.59	В .
	ATOM	392	N	THR	67	37.514				
								59.963	1.00 30.96	В
	MOTA	393	CA	THR	67	36.854	-14.420	58.662	1.00 31.82	В
	MOTA	394	CB	THR	67	36.083	-15.742	58.418	1.00 31.49	В
	MOTA	395	OG1	THR	67	36.983		58.543	1.00 35.18	В
40										
70	MOTA	396	CG2		67	35.482		57.016	1.00 30.30	В
	MOTA	397	С	THR	67	35.873	-13.252	58.565	1.00 31.85	В
	ATOM	398	0	THR	67	35.100	-12 996	59.504	1.00 32.04	В
	ATOM	399	N							
				PHE	68	35.923		57.442	1.00 29.70	В
	ATOM	400	CA	PHE	68	35.029	-11.400	57.203	1.00 31.18	`B
45	MOTA	401	CB	PHE	68	35.785	-10.063	57.305	1.00 29.26	В
	ATOM	402	CG	PHE	68.	36.374				
							-9.797	58.658	1.00 27.25	В
	MOTA	403	CD1	PHE	68	37.617	-10.309	59.001	1.00 28.36	В
	MOTA	404	CD2	PHE	68	35.666	-9.071	59.611	1.00 28.98	В
	ATOM	405	CE1		68		-10.110	60.277	1.00 27.66	
50										В
50	MOTA	406	CE2		68	36.188	-8.867	60.894	1.00 27.30	В
	MOTA	407	CZ	PHE	68	37.430	-9.388	61.225	1.00 26.68	В
	MOTA	408	С	PHE	68	34.418	-11.527	55.815	1.00 30.88	В
	ATOM	409	ō	PHE	68		-12.385	55.032		
									1.00 32.33	В
e e	ATOM	410	N	ASP	69	33.452	-10.670	55.514	1.00 30.45	В
55	ATOM	411	CA	ASP	69	32.796	-10.702	54.212	1.00 31.77	В
	MOTA	412	CB	ASP '	69	31.636	-9.698	54.185	1.00 33.60	В
	MOTA	413	CG	ASP	69	30.590	-9.988	55.258	1.00 36.34	В
	ATOM	414	OD1	ASP	69	30.514	-9.221	56.254	1.00 35.89	В
	MOTA	415	OD2		69	29.856		55.112	1.00 33.96	В
60										
55	ATOM	416	C	ASP	69	33.775		53.078	1.00 30.67	В
	ATOM	417	0	ASP	69	33.594 -	-10.882	51.970	1.00 31.26	В
	MOTA	418	N	MET	70	34.816	-9.646	53.377	1.00 31.20	В
	ATOM	419	CA	MET	70	35.836				
							-9.294	52.394	1.00 31.00	В
C E	MOTA	420	CB	MET	70	35.396	-8.081	51.567	1.00 33.24	В
65	MOTA	421	CG	MET	70	34.253	-8.330	50.598	1.00 35.15	В
	ATOM	422	SD	MET	70					
						33.994	-6.921	49.476	1.00 43.03	В
	MOTA	423	CE	MET	70	32.288	-6.531	49.777	1.00 42.27	В
	MOTA	424	С	MET	70	37.158	-8.978	53.090	1.00 29.72	В
	MOTA	425		MET	70	37.186	-8.682	54.271		
70									1.00 29.23	В
, 0	MOTA	426	N	VAL	71	38.257	-9.052	52.353	1.00 28.80	В
	MOTA	427	CA	VAL	71	39.561	-8.765	52.929	1.00 30.15	В
	ATOM	428	CB	VAL	71		-10.054	53.443	1.00 31.84	
										В
	MOTA	429	CG1	VAL	71	41.603	-9.713	54.060	1.00 33.61	В

	ATOM	430	CC2	VAL	71	39 388	-10.738	54.471	1.00 31.83	В
	MOTA	431	C	VAL	71	40.439	-8.102	51.878	1.00 29.25	В
	MOTA	432	0	VAL	71	40.471	-8.526	50.734	1.00 30.25	В
	ATOM	433	N	PHE	72	41.146	-7.053	52.285	1.00 30.15	В
5										
9	MOTA	434	CA	PHE	72	42.015	-6.306	51.384	1.00 30.67	₿
	MOTA	435	CB	PHE	72	41.445	-4.905	51.152	1.00 28.16	В
	ATOM.	436	CG	PHE	72	40.060	~4.903	50.573	1.00 27.42	В
	MOTA	437	CD1	PHE	72	39.854	-5.145	49.220	1.00 26.23	В
	MOTA	438	CD2	PHE	72	38.955	-4-686	51.390	1.00 26.64	В
10		439			72					
10	MOTA		CE1	PHE		38.565	-5.171	48.688	1.00 25.66	В
	ATOM	440	. CE2	PHE	72	37.664	-4.709	50.868	1.00 25.86	В
	MOTA	441	CZ	PHE	72	37.469	-4.954	49.516	1.00 24.73	В
		442					-6.188			
	MOTA		С	PHE	72	43.428		51.940	1.00 31.84	В
	MOTA	443	0	PHE	72	43.646	-5.560	52.973	1.00 30.82	В
15	ATOM	444	N	GLY	73	44.385	-6.797	51.247	1.00 32.27	В
	ATOM	445	CA	GLY	73	45.757	-6.727	51.697	1.00 32.67	В
	ATOM	446	С	GLY	73	46.358	-5.377	51.366	1.00 33.72	В
	MOTA	447	0	GLY	73	45.730	-4.553	50707	1.00 33.21	В
20 .	MOTA	448	N	ALA	74	47.589	-5.163	51.815	1.00 34.20	В
20 1	MOTA	449	CA	ALA	74	48.296	-3.911	51.583	1.00 35.80	. B
	ATOM	450	CB	ALA	74	49.615	-3.929	52.329	1.00 35.10	В
	MOTA	451	С	ALA	74	48.547	-3.664	50.100	1.00 37.02	В.
	ATOM	452	0	ALA	74	49.235	-2.734	49.730	1.00 38.45	В
	ATOM	453	N	SER	75	47.971	-4.498	49.250	1.00 38.40	·B
25										
23	MOTA	454	CA	SER	75	48.179	-4.356	47.821	1.00 40.23	В
	MOTA	455	СВ	SER	75	48.437	-5.733	47.204	1.00 40.06	В
	MOTA	456	OG	SER	75	47.371	-6.617	47.504	1.00 38.50	В
	MOTA	457	С	SER	75 .	46.990	-3.701	47.126	1.00 40.71	В
	ATOM	458	0	SER	75	47.155	-3.026	46.109	1.00 40.44	В
30	ATOM	459	N	THR	76	45.795	-3.917	47.677	1.00 40.56	В
-										
	MOTA	460	CA	THR	76	44.568	-3.365	47.107	1.00 40.11	В
	MOTA	461	CB	THR	76	43.325	-3.769	47.960	1.00 41.15	В
	ATOM	462	OG1	THR	76	43.690	-3.865	49.342	1.00 43.22	В
25.	MOTA	463	CG2	THR	76	42.774	-5.118	47.498	1.00 43.01	В
35	MOTA	. 464	С	THR	76	44.615	-1.849	46.937	1.00 38.50	В
	MOTA	465	0	THR	76	45.071	-1.119	47.819	1.00 38.53	В
•	-									
	MOTA	466	N	LYS	77	44.152	-1.385	45.785	1.00 36.21	В
	MOTA	467	CA	LYS	77	44.135	0.036	45.483	1.00 34.26	В
	ATOM	468	CB	LYS	77	44.482	0.243	44.011	1.00 36.10	В
40										
40	MOTA	469	CG	LYS	77	45.901	-0.174	43.651	1.00 39.66	В
	MOTA	470	CD	LYS	77	46.138	-0.013	42.153	1.00 43.10	В
	ATOM	471	CE	LYS	77					
						47.538	-0.446	41.749	1.00 44.09	В
	MOTA	472	NZ	LYS	77	47.693	-0.451	40.261	1.00 46.93	В
	MOTA	473	С	LYS	77	42.776	0.662	45.799	1.00 32.74	В
45	ATOM	474	Ō	LYS	77	41.807	-0.045	46.049		В
1.5									1.00 30.61	
	MOTA	475	N	GLN	78	42.729	1.994	45.800	1.00 31.08	В
	ATOM	476	CA	GLN	78	41.499	2.731	46.084	1.00 29.81	В
	ATOM	477	СВ	GLN	78	41.718	4.241	45.896	1.00 29.96	В
50	MOTA	478	CG	GLN	78	42.791	4.867	46.790	1.00 28.93	В
50	MOTA	479	CD	GLN	78	42.339	5.029	48.224	1.00 28.69	В
	MOTA	480	OE1	GLN	· 78	41.731	4.136	48.789	1.00 28.17	В
	MOTA	481		GLN	78	42.647	6.177	48.822	1.00 28.63	В
	ATOM	482	С	GLN	78	40.371	2.273	45.160	1.00 29.13	В
	ATOM	483	0	GLN	78	39.255	2.045	45.597	1.00 28.04	В
55										
JJ	ATOM	484	N	ILE	79	40.687	2.140	43.877	1.00 27.65	В
	MOTA	485	CA	ILE	79	39.710	1.730	42.874	1.00 28.90	В
	MOTA	486	CB	ILE	79	40.369	1.664	41.472	1.00 28.34	В
	MOTA	487	CG2		79	41.411	0.564	41.442	1.00 30.45	В.
	MOTA	488	CG1	ILE	79	39.316	1.396	40.400	1.00 29.43	В
60	MOTA	489	CD1	TLE	79	38.333	2.517	40.226	1.00 30.66	В
	MOTA	490	Ç	ILE	79	39.055	0.377	43.191	1.00 28.47	В
	MOTA	491	0	ILE	79	37.867	0.175	42.938	1.00 27.79	В
	ATOM	492	N	ASP	80	39.829	-0.548	43.749	1.00 28.15	В
CE	MOTA	493	ÇA	ASP	80	39.296	-1.866	44.076	1.00 27.60	В
65	MOTA	494	CB	ASP	80	40.435	-2.865	44.316	1.00 27.34	В
	MOTA	495	CG	ASP	80	41.439	-2.908	43.164	1.00 29.59	В
	MOTA	496	OD1		80	41.018	-2.784	41.987	1.00 27.17	В
	ATOM	497	OD2	ASP	80	42.648	-3.078	43.445	1.00 29.79	В
	MOTA	498	c	ASP	80	38.395	-1.800	45.303	1.00 27.71	В
70										
10	MOTA	499	0	ASP	80	37.394	-2.492	45.383	1.00 27.27	В
	MOTA	500	N	VAL	81	38.761	-0.964	46.265	1.00 28.05	В
	ATOM	501	CA	VAL	81	37.947	-0.820	47.460		
									1.00 27.29	В
	MOTA	502	CB	VAL	81	38.618	0.115	48.495	1.00 25.22	В

	MOTA	503	001	VAL	0.1	27 662	0.394	49.633	1.00 21.33	ъ
	ATUM	203	CGI	VAL	81	37.662	0.394			В
	MOTA	504	CG2	VAL	81	39.890	-0.532	49.036	1.00 23.97	В .
	MOTA	505	С	VAL	81	36.588	-0.244	47.079	1.00 28.97	В
	MOTA	506	0	VAL	81	35.555	-0.682	47.590	1.00 29.68	В
-										
5	ATOM	507	N	TYR	82	36.593	0.721	46.162	1.00 28.62	В
									1 00 30 03	
	MOTA	508	CA	TYR	82	35.364	1.368	45.723	1.00 30.02	В
	MOTA	509	CB	TYR	82	35.693	2.640	44.924	1.00 31.49	В.
	MOTA	510	CG	TYR	82	34.472	3.389	44.443	1.00 33.00	В
	MOTA	511	CDI	TYR	82	33.934	3.144	43.180	1.00 34.00	В
10	MOTA	512	CE1	TYR	82	32.776	3.781	42.762	1.00 37.72	В
10										•
	MOTA	513	CD2	TYR	82	33.817	4.299	45.278	1.00 32.60	• В
	ATOM	514	CE2	TYR	82	32.659	4.938	44.871	1.00 36.04	В
	MOTA	515	CZ	TYR	82	32.142	4.676	43.613	1.00 39.42	В
	ATOM	516	OH	TYR	82	30.992	5.316	43.203	1.00 42.75	В
15										
IJ	MOTA	517	С	TYR	82	34.456	0.451	44.906	1.00 30.88	В
	MOTA	518	0	TYR	82	33.264	0.363	45.168	1.00 30.76	В
	MOTA	519	N	ARG	83	35.021	-0.223	43.910	1.00 32.85	В
	MOTA	520	CA	ARG	83	34.239	-1.136	43.077	1.00 34.09	В
	MOTA	521	CB	ARG	83	35.120	-1.702	41.965	1.00 35.60	В
20										
20	ATOM	522	CG	ARG	83	35.333	-0.749	40.798	1.00 42.48	В
	ATOM	523	CD	ARG	83	36.652	-1.013	40.072	1.00 46.99	В
	MOTA	524	NE	ARG	83	36.734	-2.358	39.503	1.00 53.06	В
	ATOM	525	CZ	ARG	83	26 100	-2.758	20 404	1 00 56 70	ъ
						36.100		38.404	1.00 56.78	В
	ATOM	526	NH1	ARG	83	35.323	-1.914	37.735	1.00 57.61	В
25										
رے	ATOM	527	NHZ	ARG	83	36.254	-4.004	37.967	1.00 57.03	В
	ATOM	528	С	ARG	83	33.630	-2.277	43.895	1.00 33.36	. в
	ATOM	529	0 .	ARG	83	32.492	-2.674	43.667	1.00 34.00	В
	MOTA		N	CED		34.390				
		530	1/4	SER	84		-2.785	44.860	1.00 31.69	В
	MOTA	531	CA	SER	84	33.956	-3.899	45.701	1.00 30.91	В
30										
JU	MOTA	532	CB	SER	84	35.180	-4.582	46.322	1.00 31.88	В
	MOTA	533	OG	SER	84	36.115	-4.951	45.324	1.00 34.36	В
	MOTA	534	С	SER	84	32.983	-3.535	46.816	1.00 30.39	В
	MOTA	535	0	SER	84	31.963	-4.195	47.007	1.00 30.60	В
	MOTA	536	N	VAL	85	33.299	-2.489	47.568	1.00 29.66	В
25										
35	MOTA	537	CA	VAL	85	32.432	-2.091	48.663	1.00 28.01	В
	MOTA	538	CB	VAL	85		-1.652			
	AIOM	220			65	33.255	-1.032	49.887	1.00 27.01	В
	MOTA	539	CG1	VAL	85	32.336	-1.128	50.971	1.00 26.26	В
	MOTA	540	CG2	VAL	85	34.080	-2.815	50.407	1.00 26.27	В
	MOTA	541	С	VAL	85	31.445	-0.983	48.337	1.00 27.47	В
40										
40	ATOM	542	0	VAL	85	30.249	-1.149	48.498	1.00 28.23	В
	MOTA	543	N	VAL	86	31.960	0.145	47.868	1.00 28.02	В
	MOTA	544	CA	VAL	86	31.132	1.313	47.585	1.00 28.51	В
	MOTA	545	CB	VAL	86	32.004	2.568	47.370	1.00 26.65	В
	MOTA	546	CG1							
4.5					86	31.180	3.808	47.625	1.00 25.89	В
45	MOTA	547	CG2	VAL	86	33.220	2.532	48.267	1.00 25.41	В
	MOTA	548	С	VAL	86	30.150	1.224	46.425	1.00 29.30	В
	MOTA	549	0	VAL	86	28.959	1.479	46.599	1.00 28.44	В
	MOTA	550	N	CYS	87	30.649	0.881	45.244	1.00 29.85	В
	MOTA	551	CA	CYS	87	29.802	0.786	44.064	1.00 33.34	В
~ ^										В
50	MOTA	552	CB	CYS	87	30.549	0.025	42.965	1.00 36.49	В
	MOTA	553	SG	CYS	87	29.936	0.313	41.286	1.00 43.07	B
	ATOM	554	С	CYS	87	28.445	0.131	44.373	1.00 34.93	В
	ATOM	555	0	CYS	87	27.396	0.670	44.026	1.00 34.18	₿
	ATOM	556	N	PRO	88	28.452	-1.035	45.045	1.00 35.57	В
55										
JJ	ATOM	557	CD	PRO	88	29.603	-1.876	45.420	1.00 37.48	В
	ATOM	558	CA	PRO		27.195	-1.715	45.378	1.00 35.50	В
							-			
	MOTA	559	CB	PRO	88	27.664	-2.989	46.078	1.00 35.52	В
	MOTA	560	CG	PRO	88	28.984	-3.247	45.464	1.00 36.85	В
	MOTA	561	С	PRO	88	26.295	-0.874	46.287	1.00 35.13	В
60										
60	ATOM	562	0	PRO	88	25.099	-0.765	46.050	1.00 35.74	В
	MOTA	563	N	ILE	89	26.885	-0.288	47.327	1.00 34.00	В
	MOTA	564	CA	ILE	89	26.140	0.535	48.279	1.00 33.52	В
	MOTA	565	CB	ILE	89	27.031	0.978	49.465	1.00 33:84	В
	ATOM	566	CG2		89	26.250		50.384	1.00 34.73	
65							1.910			
65	MOTA	567	CG1	ILE	89	27.514	-0.247	50.243	1.00 33.35	В
	MOTA	568	CD1	ILE	89	28.486	0.077	51.357	1.00 33.52	В
	ATOM	569	С	ILE	89	25.552	1.786	47.636	1.00 32.98	В
	MOTA	570	0	ILE	89	24.485	2.243	48.016	1.00 33.67	В
			N		90				1.00 32.32	
70	MOTA	571		LEU		26.258	2.341	46.662		В
70	MOTA	572	CA	LEU	90	25.782	3.540	45.996	1.00 32.57	В
. –										
	ATOM	573	СB	LEU	90	26.866	4.097	45.074	1.00 30.54	В
	ATOM									
		574	CG	LEU	90	26.431	5.292	44.229	1.00 29.69	В
	MOTA	575	CD1	LEU	90	26.018	6.448	45.122	1.00 28.62	В
					- -					-

	MOTA	576	CD2	LEU	90	27.564	5.695	43.319	1.00 31.53	В
•										
	MOTA	577	С	LEU	90	24.504	3.272	45.202	1.00 32.92	В
	ATOM	578	0	LEU	90	23.567	4.074	45.240	1.00 32.45	В
	MOTA	579	N	ASP	91	24.466	2.147	44.491	1.00 33.45	В
5										
5	ATOM	580	CA	ASP	91	23.292	1.785	43.699	1.00 34.72	В
	MOTA	581	CB	ASP	91	23.520	0.470	42.940	1.00 35.65	В
	ATOM		CG		91					
		582		ASP		24.593	0.582	41.863	1.00 39.61	В
	MOTA	583	OD1	ASP	91	24.686	1.648	41.214	1.00 40.33	В
	MOTA	584	OD2	ACD	91	25.335	-0.409	41.661	1.00 41.38	В
10										
10	MOTA	585	C	ASP	91	22.068	1.633	44.597	1.00 33.10	В
	MOTA	586	.0	ASP	91	20.954	1.885	44.174	1.00 33.56	В
	MOTA	587	N	GLU	92	22.290	1.221	45.839	1.00 32.56	В
	ATOM	588	CA	GLU	92	21.196	1.044	.46.783	1.00 34.16	В
	ATOM	589	CB	GLU	92	21.657	0.171	47.954	1.00 37.44	В
15		590					-0.258			
15	MOTA		CG	GLU	92	20.545		48.890	1.00 42.74	В
	ATOM	591	CD	GLU	92	20.880	-1.536	49.648	1.00 46.50	В
•	ATOM	592	OE1	GLU	92	20.053	-1.956	50.490	1.00 47.07	В
	MOTA	593		GLU	92	21.962	-2.120	49396	1.00 46.74	В
:	MOTA	594	С	GLU	92	20.709	2.409	47.280	1.00 32.53	В
20 1	MOTA	595	0	GLU	92	19.518	2.608	47.519	1.00 30.70	В
	MOTA	596	N	VAL	93	21.641	3.348	47.422	1.00 31.20	В
	MOTA	597	CA	VAL	93	21.303	4.699	47.854	1.00 31.28	В
	MOTA	598	CB	VAL	93	22.580	5.569	48.076	1.00 31.49	В
									•	
05	MOTA	. 599	CG1		93	22.194	7.010	48.365	1.00 27.40	·B
25	MOTA	600	CG2	VAL	93	23.398	5.004	49.233	1.00 33.28	В
	MOTA	601	C	VAL	93	20.452	5.322	46.750	1.00 29.79	В
	MOTA	602	0	VAL	93	19.416	5.913	47.013	1.00 28.28	В
	MOTA	603	N	ILE	94	20 ⁻ .899	5.163	45.510	1.00 27.82	В
	MOTA	604	CA	ILE	94	20.166	5.703	44.378	1.00 30.44	. B
20										
30	MOTA	605	CB	ILE	94	20.915	5.429	43.051	1.00 28.59	В
	MOTA	606	CG2	ILE	94	20.035	5.787	41.853	1.00 26.78	В
		607	CG1		94					
	MOTA					22.216	6.240	43.037	1.00 27.01	В
	MOTA	608	CD1	ILE	94	23.087	5.978	41.846	1.00 26.60	В
	MOTA	609	С	ILE	94	18.749	5.131	44.306	1.00 32.32	В
35	MOTA			ILE	94	17.872		43.714		
55			0				5.738		1.00 32.23	В
	MOTA	611	N	MET	95	18.531	3.968	44.920	1.00 34.51	В
	MOTA	612	CA	MET	95	17.201	3.360	44.923	1.00 36.17	В
	MOTA	613	СВ	MET	95	17.282	1.850	45.149	1.00 38.61	В
	MOTA	614	CG	MET	95	17.372	1.017	43.881	1.00 40.44	В
40	ATOM	615	SD	MET	95	17.488	-0.772	44.242	1.00 46.46	В
•	MOTA	616	CE	MET	95	19.102	-1.171	43.546	1.00 44.51	В
	ATOM	617	С	MET	95	16.315	3.979	45.996	1.00 36.50	В
	ATOM	618	ō	MET	95	15.113	3.732	46.030	1.00 37.42	В
4-	ATOM	619	N	GLY	96	16.914	4.775	46.879	1.00 36.28	В
45	MOTA	620	CA	GLY	96	16.145	5.414	47.932	1.00 35.74	В
	ATOM	621	C	GLY	96	16.366	4.830	49.314	1.00 36.78	В
	MOTA	622	0	GLY	96	15.538	5.026	50.210	1.00 37.90	В
	ATOM	623	N	TYR	97	17.479	4.118	49.487	1.00 36.85	В
	ATOM	624	CA	TYR	97	17.835	3.496	50.763	1.00 37.58	В
50										
<i>3</i> 0	ATOM	625	СВ	TYR	97	18.381	2.081	50.525	1.00 40.65	В
	MOTA	626	CG	TYR	97	17.341	1.025	50.217	1.00 45.13	В
	MOTA	627	CD1		97	16.518	0.518	51.220	1.00 46.62	В
	MOTA	628	CE1	TYR	97	15.558	-0.454	50.944	1.00 49.26	В
	ATOM	629	CD2	TYR	97	17.182	0.533	48.921	1.00 46.06	В
55	MOTA	630	CE2		97	16.228	-0.436	48.630	1.00 49.09	В
55										
	MOTA	631	CZ	TYR	97	15.417	-0.928	49.646	1.00 50.42	В
	ATOM	632	он	TYR	97	14.465	-1.888	49.358	1.00 52.50	В
	MOTA	633	C		97	18.889	4.304	51.526	1.00 35.44	
				TYR						₿
	MOTA	634	0	TYR	97	19.789	4.876	50.926	1.00 37.02	В
60 ·	MOTA	635	N	ASN	98	18.776	4.349	52.849	1.00 31.97	В
	MOTA	636			98		5.059			
			CA	ASN		19.759		53.662	1.00 30.42	₿
	ATOM	637	CB	ASN	98	19.169	5.460	55.025	1.00 30.64	В
	MOTA	638	CG	ASN	98	18.239	6.663	54.945	1.00 28.74	В
45	ATOM	639	OD1		98	18.255	7.413	53.981	1.00 29.47	В
65	ATOM	640	ND2	ASN	98	17.436	6.855	55.984	1.00 27.34	В
	ATOM	641	C	ASN	98	20.942	4.124			
								53.897	1.00 29.81	В
	ATOM	642	0	ASN	98	20.762	3.006	54.324	1.00 29.82	В
	ATOM	643	N	CYS	99	22.152	4.590	53.615	1.00 28.53	В
	ATOM	644	CA	CYS	99	23.339	3.767		1.00 26.90	
70								53.816		В
70	MOTA	645	CB	CYS	99	23.974	3.384	52.477	1.00 28.87	В
	MOTA	646	SG	CYS	99	22.946	2.349	51.428	1.00 34.21	В
	ATOM									
		647	С	CYS	99	24.382	4.465	54.677	1.00 25.00	В
	MOTA	648	0	CYS	99	24.380	5.670	54.830	1.00 25.25	В

	ATOM	649	N	THR	100	25.285	3.671	55.232	1.00 23.32	В
	MOTA	650	CA	THR	100	26.341	4.187	56.080	1.00 19.59	В
	ATOM	651	CB	THR	100	25.876	4.258	57.544	1.00 17.10	В
5	ATOM	652		THR	100	24.789	5.179	57.657	1.00 16.21	В
5	ATOM	653	CG2	THR	100	27.005	4.696	58.456	1.00 15.27	В
	ATOM .	654 655	c o	THR THR	100 - 100	27.552	3.266 2.039	55.982 56.005	1.00 21.18	· В В
	MOTA	656	И	ILE	101	27.417 28.732	3.858	55.849	1.00 22.70 1.00 18.53	В
	MOTA	657	CA	ILE	101	29.967		55.782	1.00 17.55	В
10	ATOM	658	CB	ILE	101	30.650	3.212	54.420	1.00 16.14	В
	ATOM	659		ILE	101	31.939	2.414	54.423	1.00 16.50	. B
	ATOM	660		ILE	101	29.730	2.690	53.318	1.00 14.57	В
	MOTA	661		ILE	101	30.186	3.077	51,930	1.00 14.45	В
1.5	MOTA	662	С	ILE	101	30.913	3.654	56.834	1.00 19.99	В
15	MOTA	663	0	ILE	101 .	31.296	4.822	56.786	1.00 20.78	В
	MOTA	664	N	PHE	102	31.273	2.808	57.793	1.00 19.14	В
	ATOM	665	CA	PHE	102	32.176	3.179	58.876	1.00 17.58	В
	MOTA	666	CB	PHE	102	31.835	2.373	60.123	1.00 17.67	В
20	MOTA	667	CG	PHE	102	30.618	2.842	60.847	1.00 17.05	В
20	MOTA MOTA	668 669		PHE	102 102	30.714 29.386	3.855 2.239	61.790 60.624	1.00 16.04	В
	MOTA	670		PHE	102	29.603	4.265	62.508	1.00 16.40 1.00 16.56	B B
	MOTA	671	CE2	PHE	102	28.268	2.643	61.337	1.00 18.62	В
	ATOM	672	cz	PHE	102	28.377	3.658	62.283	1.00 16.81	В
25	MOTA	673	С	PHE	102	33.625	2.891	58.515	1.00 16.69	В
	MOTA	674	0	PHE	102	33.910	2.289	57.516	1.00 18.17	. в
	MOTA	675	N	ALA.	103	34.535	3.338	59.366	1.00 17.68	В
	MOTA	676	CA	ALA	103	35.961	3.089	59.187	1.00 17.02	В
20	MOTA	677	CB	ALA	103	36.620	4.229	58.451	1.00 16.82	В
30	MOTA	678	C	ALA	103	36.471	2.991	60.617	1.00 17.64	В
	MOTA	679	0	ALA	103	36.482	3.963	61.339	1.00 18.79	В
	MOTA MOTA	680 681	N CA	TYR TYR	104 104	36.866 37.340	1.786 1.540	61.012	1.00 18.22	В
	ATOM	682	CB	TYR	104	36.436	0.496	62.368 63.034	1.00 16.40 1.00 15.83	B B
35	MOTA	683	CG	TYR	104	36.706	0.291	64.508	1.00 13.63	В.
-	MOTA	684		TYR	104	37.771	-0.501	64.941	1.00 10.95	В
	MOTA	685	CE1	TYR	104	38.046	-0.659	66.301	1.00 11.52	В
	MOTA	686	CD2	TYR	104	35.919	0.920	65.469	1.00 10.91	В
40	MOTA	687	CE2	TYR	104	36.187	0.768	66.832	1.00 12.42	В
40	MOTA	688	CZ	TYR	104	37.253	-0.023	67.239	1.00 10.32	В
	MOTA	689	ОН	TYR	104	37.526	-0.180	68.574	1.00 11.99	В
	MOTA	690	C	TYR	104	38.778	1.061	62.380	1.00 15.64	В
	MOTA	691	0	TYR	104	39.203	0.348	61.497	1.00 17.51	В
45	ATOM ATOM	692 693	N CA	GLY GLY	105	39.524	1.456	63.397	1.00 15.78	В
73	ATOM	694	C	GLY	105 105	40.904 41.748	1.047 2.044	63.475 64.226	1.00 16.05 1.00 16.81	B B
	MOTA	695	õ	GLY	105	41.318	3.151	64.526	1.00 19.22	В
	MOTA	696	N	GLN	106	42.963	1.616	64.531	1.00 19.22	В
	ATOM	697	CA	GLN	106	43.940	2.408	65.244	1.00 18.74	В
50	ATOM	698	CB	GLN	106	45.122	1.519	65.652	1.00 19.69	В
	MOTA	699	CG	GLN	106	46.278	2.251	66.305	1.00 23.87	В
	MOTA	700	CD	GLN	106	47.527	1.411	66.407	1.00 24.14	В
	ATOM	701	OE1		106	47.865	0.669	65.490	1.00 27.37	В
55	ATOM	702	NE2		106	48.225	1.528	67.525	1.00 25.29	В
33	MOTA	703	C	GLN	106	44.440	3.552	64.363	1.00 20.10	В
	MOTA	704	0	GLN	106	44.438	3.451	63.134	1.00 19.09	В
	ATOM ATOM	705 706	N CA	THR THR	107 107	44.864 45.385	4.639 5.792	65.004 64.291	1.00 19.11 1.00 18.65	В
	MOTA	707	CB	THR	107	45.849	6.914	65.270	1.00 18.65	B B
60	ATOM	708	OG1		107	44.730	7.405	66.017	1.00 19.66	В
	MOTA	709	CG2		107	46.476	8.064	64.497	1.00 15.96	В
	MOTA	710	C	THR	107	46.588	5.391	63.439	1.00 17.71	В
	MOTA	711	0	THR	107	47.518	4.747	63.921	1.00 16.56	В
	ATOM	712	N	GLY	108	46.554	5.786	62.171	1.00 17.28	В
65	MOTA	713	CA	GLY	108	47.642	5.483	61.267	1.00 15.71	В
	MOTA	714	C	GLY	108	47.499	4.181	60.505	1.00 17.55	В
	MOTA	715	0	GLY	108	48.489	3.682	59.938	1.00 17.87	В
	ATOM	716	N	THR	109	46.288	3.626	60.478	1.00 15.83	В
70	ATOM	717	CA	THR	109	46.064	2.374	59.765	1.00 14.74	В
, ,	MOTA MOTA	718 719	CB OG1	THR	109 109	45.276 43.978	1.352 1.866	60.632	1.00 13.57 1.00 13.63	В
	ATOM	720	CG2	THR	109	45.978	1.064	60.943 61.934	1.00 13.63	B B
	ATOM	721	C	THR	109	45.350	2.573	58.435	1.00 12.00	В
										_

	ATOM	722	0	THR	109	45.132	1.602	57.708	1.00 14.55	В
	MOTA	723	N	GLY	110	44.977	3.819	58.124	1.00 13.70	В
	ATOM	724	CA	GLY	110	44.321	4.073	56.849	1.00 10.56	В
	ATOM	725	c	GLY	110	42.846	4.433	56.833	1.00 10.76	В
5	MOTA	726	Ö	GLY	110	42.201	4.298	55.792		В
,										
	MOTA	727	N	LYS	111	42.302	4.885	57.959	1.00 8.99	В
	ATOM	728	CA	LYS	111	40.889	5.267	58.022	1.00 11.48	В
	MOTA	729	CB	LYS	111	40.497	5.693	59.449	1.00 12.59	В
10	MOTA	730	CG	LYS	111	40.315	4.531	60.426	1.00 15.28	В
10	MOTA	731	CD	LYS	111	39.651	4.955	61.738	1.00 12.73	В
	ATOM	732	·CE	LYS	111	40.439	6.034	62.455	1.00 11.56	В
	MOTA	733	NZ	LYS	111	41.905	5.766	62.396	1.00 10.51	В
	MOTA	734	С	LYS	111	40.575	6.408	57.062	1.00 13.97	В
,	ATOM	735	Ō	LYS	111	39.683	6.302	56.206	1.00 15.37	В
15	ATOM	736	N	THR	112	41.321	7.498	57.198	1.00 13.82	В
	ATOM	737	CA	THR	112	41.120	8.663	56.353	1.00 12.58	В
	MOTA	738	CB	THR	112	41.895	9.871	56.926	1.00 12.79	В
	ATOM	739								
			OG1		112	41.408	10.160	58.245	1.00 9.63	В
20	MOTA	740		THR	112	41.723	11.103	56.037	1.00 10.46	В
20	ATOM	741	C	THR	112	41.535	8.396	54.905	1.00 14.40	. В
	MOTA	742	0	THR	112	40.886	8.846	53.978	1.00 15.19	В
	MOTA	743	N	PHE	113	42.618	7.651	54.723	1.00 15.74	В.
	MOTA	744	CA	PHE	113	43.095	7.326	53.384	1.00 17.09	В
25	ATOM	745	СВ	PHE	113	44.316	6.408	53.463	1.00 17.69	·B
25	MOTA	746	CG	PHE	113	44.867	6.030	52.123	1.00 20.87	В
	MOTA	747	CD1	PHE	113	45.783	6.849	51.475	1.00 22.41	В
	MOTA	748	CD2	PHE	113	44.445	4.871	51.490	1.00 22.63	B
	MOTA	749	CE1	PHE	113	46.271	6.517	50.218	1.00 22.81	В
	MOTA	750	CE2	PHE	113	44.924	4.529	50.228	1.00 23.87	. в
30	MOTA	751	ĊZ	PHE	113	45.840	5.354	49.590	1.00 25.27	В
	MOTA	752	С	PHE	113	42.000	6.626	52.580	1.00 18.62	В
	MOTA	753	0	PHE	113	41.817	6.888	51.389	1.00 17.60	В
•	ATOM	754	N	THR	114	41.291	5.719	53.247	1.00 19.63	В
	MOTA	755		THR	114	40.212	4.945	52.646	1.00 18.57	В
35 °	ATOM	756		THR	114	39.816	3.760	53.582	1.00 20.30	В
	ATOM	757	OG1		114	40.970	2.947	53.828	1.00 18.79	В
	ATOM	758	CG2		114	38.700	2.910	52.972	1.00 12.74	В
	ATOM	759	c	THR	114		5.825	52.410	1.00 19.70	B
	MOTA	760		THR	114	38.497	5.932	51.297	1.00 22.13	В
40	MOTA	761		MET	115	38.518	6.473	53.465	1.00 19.43	В
	MOTA	762		MET	115	37.345	7.318	53.347	1.00 20.55	
	ATOM	763		MET	115	36.877	7.771	54.730		В
	MOTA	764		MET	115	36.471			1.00 21.97	В
	MOTA	765					6.620	55.644	1.00 27.07	В
45				MET	115	35.328	5.432	54.848	1.00 29.66	В
73	MOTA	766		MET	115	33.753	6.265	55.089	1.00 27.98	В
	ATOM	767		MET	115	37.532	8.528	52.454	1.00 21.26	В
	MOTA	768		MET	115	36.639	8.866	51.674	1.00 23.74	В
	ATOM	769		GLU	116	38.687	9.179	52.549	1.00 20.10	В
50	ATOM	7.70		GLU	116	38.937	10.377	51.749	1.00 20.30	В
50	MOTA	771		GLU	116	39.323	11.541	52.659	1.00 19.03	В
	MOTA	772	_	GLU	116	38.309	11.824	53.741	1.00 17.09	В
	MOTA	773		GLU	116	38.746	12.922	54.687	1.00 18.90	В
	MOTA	774	OE1	GLU	116	39.886	13.421	54.550	1.00 21.39	В
~ ~	MOTA	775	OE2	GLU	116	37.951	13.280	55.579	1.00 17.52	В
55	MOTA	776	С	GLU	116	40.010	10.194	50.694	1.00 20.60	В
	ATOM	777	0	GLU	116	39.804	10.494	49.527	1.00 19.26	В
	ATOM	778	N	GLY	117	41.166	9.708	51.116	1.00 22.39	В
	MOTA	779		GLY	117	42.249	9.508	50.176	1.00 24.67	В.
	MOTA	780		GLY	117	43.194	10.689	50.144	1.00 25.76	В
60	ATOM	781		GLY	117	43.056	11.630	50.918	1.00 24.17	В
	ATOM	782		GLU	118	44.162	10.635	49.237	1.00 27.49	В
	ATOM	783		GLU	118	45.133	11.710	49.128	1.00 28.73	B
	ATOM	784		GLU	118	46.465	11.273	49.740	1.00 30.64	В
	ATOM	785		GLU	118	46.311	10.255	50.853	1.00 35.23	В
65	MOTA	786		GLU	118	47.579	10.255	51.657	1.00 35.23	
J J	ATOM	787	OE1		118	48.671	9.993			В
								51.049	1.00 35.58	В
	MOTA	788	OE2		118	47.476	9.958	52.900	1.00 40.04	В
	ATOM	789		GLU	118	45.338	12.082	47.671	1.00 27.97	В
70	ATOM	790		GLU	118	44.692	11.542	46.779	1.00 29.50	В
/0	MOTA	791		ARG	119	46.244	13.017	47.436	1.00 25.87	В
	MOTA	792		ARG	119	46.532	13.439	46.085	1.00 25.52	В
	MOTA	793		ARG	119	46.613	14.968	46.006	1.00 24.48	В
	MOTA	794	CG	ARG	119	45.323	15.708	46.358	1.00 23.62	. В

	MOTA	795	CD	ARG	119	44.190	15.361	45.387	1.00 22.16	В
	MOTA	796	NE	ARG	119	44.654	15.191	44.011	1.00 20.25	В
	MOTA	797	CZ	ARG	119	44.382	16.018	43.005	1.00 19.31	В
	MOTA	798	NH1	ARG	119	43.642	17.102	43.203	1.00 19.24	В
5	ATOM	799	NH2		119	44.842	15.744	41.791	1.00 17.50	В
9										
	ATOM .	800	C	ARG	119	47.857	12.836	45.654	1.00 26.80	В
	ATOM	801	0	ARG	119	48.779	12.711	46.457	1.00 25.89	В
	MOTA	802	N	SER	120	47.942	12.440	44.390	1.00 25.98	В
	ATOM	803	CA	SER	120	49.189	11.893	43.880	1.00 28.78	В
10										
10	MOTA	804	CB	SER	120	49.015	11.326	42.472	1.00 29.79	В
	ATOM	805	OG	SER	120	48.428	10.038	42.508	1.00 33.26	• В
	MOTA	806	С	SER	120	50.130	13.077	43.834	1.00 27.18	В
	ATOM	807	ŏ	SER	120	49.779	14.121	43.326	1.00 27.97	В
16	MOTA	808	N	PRO	121	51.348	12.913	44.357	1.00 27.06	В
15	MOTA	809	CD	PRO	121	51. 9 02	11.662	44.900	1.00 26.17	В
	ATOM	810	CA	PRO	121 .	52.350	13.987	44.381	1.00 27.66	В
	MOTA	811	CB	PRO	121	53.528	13.342	45.117	1.00 27.55	. В
			CG	PRO	121	53.386		44.779		
	MOTA	812					11.899		1.00 28.94	В
20	ATOM	813	С	PRO	121	52.760	14.591	43.031	1.00 27.47	В
20	ATOM	814	0	PRO	121	52.773	13.914	42.009	1.00 27.14	В
	ATOM	815	N	ASN	122	. 53.072	15.885	43.050	1.00 27.34	В
	ATOM	816		ASN	122	53.517	16.615	41.865	1.00 28.41	В
	MOTA	817		ASN	122	54.690	15.875	41.217	1.00 29.21	В
~ =	MOTA	818	CG	ASN	122	55.857	16.789	40.906	1.00 29.30	В
25	MOTA	819	OD1	ASN	122	56.355	17.491	41.777	1.00 30.37	В
	MOTA	820	ND2		122	56.305	16.774	39.656	1.00 30.61	. в
									1.00 28.67	
	MOTA	821		ASN	122	52.434	16.859	40.817		В
	MOTA	822		ASN	122	52.725	16.940	39.627	1.00 25.87	В
	MOTA	823	N	GLU	123	51.191	16.985	41.265	1.00 30.12	В
30	ATOM	824	CA	GLU	123	50.070	17.240	40.356	1.00 33.32	В
	MOTA	825		GLU	123	50.105	18.699	39.870	1.00 33.54	В
	MOTA	826		GLU	123	50.037	19.748	40.968	1.00 33.76	В
	MOTA	827	CD	GLU	123	49.872	21.158	40.420	1.00 34.11	В
	ATOM	828	OE1	GLU	123	50.763	21.623	39.678	1.00 32.71	В
35	MOTA	829	OE2	GLU	123	48.848	21.804	40.734	1.00 33.32	В.
	ATOM	830		GLU	123	50.061	16.307	39.137	1.00 34.30	В
	ATOM	831		GLU	123	49.856	16.743	38.013	1.00 32.10	В
	ATOM	832	N	GLU	124	50.283	15.020	39.373	1.00 36.35	В
	ATOM	833	CA	GLU	124	50.303	14.046	38.292	1.00 36.52	В
40	MOTA	834		GLU	124	50.709	12.678	38.846	1.00 40.35	B
••										
	MOTA	835		GLU	124	51.279	11.711	37.815	1.00 45.05	В
	MOTA	836		GLU	124	52.026	10.550	38.458	1.00 47.77	В
	MOTA	837	OE1	GLU	124	51.966	10.427	39.705	1.00 47.83	В
	ATOM	838	OE2	GLU	124	52.671	9.769	37.720	1.00 48.04	В
45	MOTA	839		GLU	124	48.942	13.964	37.590	1.00 36.15	· B
75										
	MOTA	840		GLU		48.876	13.987	36.363	1.00 34.16	В
	MOTA	841	N	TYR	125	47.859	13.886	38.361	1.00 35.31	В
	MOTA	842	CA	TYR	125	46.524	13.803	37.770	1.00 36.12	В
	ATOM	843		TYR	125	45.863	12.440	38.054	1.00 38.61	В
50		844								
50	MOTA			TYR	125	46.757	11.216	37.992	1.00 39.31	В
	MOTA	845	CD1		125	47.657	10.933	39.019	1.00 39.77	В
	MOTA	846	CE1	TYR	125	48.454	9.784	38.987	1.00 40.96	В
	MOTA	· 847	CD2	TYR	125	46.675	10.321	36.922	1.00 39.64	В
	MOTA	848		TYR	125	47.468	9.169	36.879	1.00 40.42	В
55		849		TYR	125				1.00 40.42	
JJ	MOTA					48.355	8.908	37.916		В
	MOTA	850	ОН	TYR	125	49.141	7.776	37.882	1.00 43.64	В
	ATOM	851	С	TYR	125	45.590	14.873	38.332	1.00 35.75	В
	ATOM	852	0	TYR	125	45.925	15.577	39.273	1.00 36.04	В
		853			126		14.976	37.729		
60	ATOM			THR		44.409			1.00 35.01	В
UU	MOTA	854	CA	THR	126	43.385	15.901	38.189	1.00 34.12	В
	MOTA	855	CB	THR	126	42.393	16.275	37.064	1.00 34.09	В
	MOTA	856	OG1		126	41.885	15.080	36.458	1.00 36.33	В
	MOTA	857	CG2		126	43.075	17.134	36.005	1.00 30.16	В
45	MOTA	858		THR	126	42.645	15.117	39.271	1.00 34.15	В
65	ATOM	859	0	THR	126	42.555	13.896	39.197	1.00 35.30	В
	MOTA	860	N	TRP	127	42.111	15.807	40.270	1.00 33.25	В
	MOTA	861		TRP	127	41.422	15.133	41.363	1.00 31.64	В
	ATOM									
		862		TRP	127	40.596	16.135	42.182	1.00 28.58	В
70	MOTA	863		TRP	127	39.362	16.610	41.489	1.00 25.55	В
70	MOTA	864	CD2	TRP	127	38.066	16.008	41.551	1.00 23.28	В
	ATOM	865	CE2	TRP	127	37.218	16.754	40.699	1.00 23.64	В
	ATOM	866	CE3		127	37.537	14.907	42.244	1.00 23.43	В
	MOTA	867	CD1	IRP	127	39.255	17.667	40.631	1.00 23.80	В

•	MOTA	868		TRP	127	37.969	17.761	40.150	1.00 24.71	В
	MOTA	869	CZ2	TRP	127	35.867	16.433	40.518	1.00 24.05	В
	MOTA MOTA	870 871	CZ3	TRP	127 127	36.192 35.372	14.585 15.351	42.065	1.00 24.74 1.00 26.04	B B
5	ATOM	872	Ċ	TRP	127	40.522	13.968	41.207 40.931	1.00 20.04	В
•	ATOM	873	õ	TRP	127	40.510	12.927	41.579	1.00 32.64	В
	MOTA		N	GLU	128	39.781	14.131	39.838	1.00 32.66	В
	MOTA	875	CA	GLU	128	38.869	13.078	39.394	1.00 33.32	В
10	ATOM	876	CB	GLU	128	37.785	13.669	38.502	1.00 34.68	В
10	MOTA	877	CG	GLU	128	38.287	14.201	37.178	1.00 39.01	В
	MOTA	878	.CD	GLU	128	37.206	14.964	36.442	1.00 42.74	В
	MOTA	879		GLU	128	36.895		36.867	1.00 44.33	В
•	MOTA MOTA	880 881		GLU GLU	128 128	36.654 39.512	14.422 11.879	35.458 38.700	1.00 43.63	В
15	ATOM	882	CO	GLU	128	38.825	10.930	38.348	1.00 32.67 1.00 31.45	B B
	MOTA	883	N	GLU	129	40.825	11.926	38.500	1.00 32.62	В
	MOTA	884	CA	GLU	129	41.532	10.815	37.871	1.00 33.28	В
	MOTA	885	CB	GLU	129	42.192	11.246	36.561	1.00 35.75	В
20	MOTA	886	CG	GLU	129	41.218	11.496	35.420	1.00 39.64	В
20	MOTA	887	CD	GLU	129	41.922	11.680	34.082	1.00 42.49	В
	MOTA	888		GLU	129	41.266	12.139	33.119	1.00 43.56	В
	ATOM	889		GLU	129	43.129	11.367	33.996	1.00 45.44	В
	ATOM ATOM	890 891	C	GLU	129 129	42.602 43.242	10.280 9.297	38.808 38.511	1.00 33.23 1.00 33.33	B ∙B
25	ATOM	892	N	ASP	130	42.776	10.934	39.951	1.00 32.98	В
	ATOM	893	CA	ASP	130	43.789	10.516	40.912	1.00 32.86	В
	MOTA	894	CB	ASP	130	43.884	11.544	42.045	1.00 34.15	В
	MOTA	895	CG	ASP	130 ·	45:247	11.564	42.699	1.00 35.32	В
20	MOTA	896		ASP	130	45.765	10.477	43.030	1.00 36.91	В
30	MOTA	897		ASP	130	45.801	12.665	42.882	1.00 36.83	В
	MOTA	898	C	ASP	130	43.468	9.129	41.485	1.00 33.07	В
	MOTA MOTA	899 900	o N	ASP PRO	130 131	42.429 44.367	8.928 8.152	42.114 41.268	1.00 32.52 1.00 32.43	B B
	MOTA	901	CD	PRO	131	45.638	8.278	40.533	1.00 32.43	В
35 ·	ATOM ·	. 902	CA	PRO	131	44.186	6.782	41.757	1.00 30.77	В
	MOTA	903	CB	PRO	131	45.339	6.029	41.102	1.00 31.15	В
	MOTA	904	CG.	PRO	131	46.399	7.073	41.005	1.00 31.37	В
	MOTA	905	Ċ	PRO	131	44.192	6.673	43.283	1.00 30.54	В
40	MOTA	906	0	PRO	131	43.717	5.688	43.845	1.00 31.07	В
40	MOTA	907	N	LEU	132	44.721	7.691	43.953	1.00 28.68	В
	MOTA MOTA	908 909	CA CB	LEU	132 132	44.750 45.965	7.684 8.461	45.407 45.918	1.00 26.49 1.00 24.68	В
	MOTA	910	CG	LEU	132	47.355	7.961	45.497	1.00 24.68	B B
	ATOM	911		LEU	132	48.414	8.782	46.221	1.00 24.29	В
45	MOTA	912	CD2		132	47.526	6.481	45.843	1.00 26.94	В
	MOTA	913	C	LEU	132	43.455	8.248	46.008	1.00 26.30	В
	MOTA	914	Ο.	LEU	132	43.294	8.285	47.228	1.00 26.84	В
	MOTA	915	N	ALA	133	42.532	8.672	45.145	1.00 24.55	В
50	ATOM ATOM	916	CA.	ALA	133 133	41.243	9.217	45.572	1.00 25.15	В
50	MOTA	917 918	CB C	ALA ALA	133	40.393 40.502	9.562 8.215	44.352 46.453	1.00 24.26 1.00 25.64	B B
	ATOM	919	ŏ	ALA	133	40.528	7.034	46.201	1.00 27.86	В
	ATOM	920	N	GLY	134	39.831	8.706	47.485	1.00 26.27	В
	ATOM	921	CA	GLY	134	39.107	7.822	48.379	1.00 24.63	В
55	MOTA	922	¢	GLY	134	37.633	7.705	48.038	1.00 24.63	В
	MOTA	923	0	GLY	134	37.176	8.224	47.013	1.00 23.91	В
	ATOM	924		ILE		36.887	7.030		1.00 22.69	В
	ATOM	925 926	CA	ILE	135	35.457	6.816	48.704	1.00 21.86	В.
60	MOTA MOTA	927	CB CG2	ILE	135 135	34.839 33.315	6.028 5.945	49.898 49.745	1.00 21.68 1.00 20.01	B B
••	ATOM	928	CG1		135	35.464	4.628	49.971	1.00 20.31	В
	ATOM	929	CD1		135	35.183	3.865	51.246	1.00 16.89	В
	MOTA	930	С	ILE	135	34.652	8.103	48.481	1.00 20.87	В
~=	MOTA	931	0	ILE	135	33.956	8.228	47.495	1.00 19.45	В
65	MOTA	932	N	ILE	136	34.762	9.053	49.405	1.00 20.74	В
	ATOM	933	CA	ILE	136	34.018	10.309	49.297	1.00 19.78	В
	MOTA	934	CB	ILE	136	34.420	11.273	50.436	1.00 19.46	В
	MOTA MOTA	935 936	CG2 CG1		136 136	33.654	12.581	50.302	1.00 23.46 1.00 19.18	В
70	MOTA	937	CD1		136	34.128 34.597	10.616 11.398	51.792 53.011	1.00 19.18	B B
· •	ATOM	938	C	ILE	136	34.146	11.016	47.929	1.00 19.32	. В
	MOTA	939	ŏ.	ILE	136	33.149	11.258	47.255	1.00 18.78	В
	MOTA	940	N	PRO	137 -	35.377	11.340	47.499	1.00 18.18	В

	ATOM	941	CD	PRO	137	36.695	11.158	48.127	1.00 15.47	В
	ATOM	942	CA	PRO	137	35.501	12.008	46.198	1.00 17.79	В
	ATOM	943	CB	PRO	137	36.995	12.321	46.105	1.00 15.58	В
	ATOM	944	CG	PRO	137	37.618	11.255	46.946	1.00 16.71	В
5	MOTA	945	Č	PRO	137	35.010	11.135	45.040	1.00 20.22	B
_	ATOM	946	ŏ	PRO	137	34.434	11.625	44.080	1.00 21.41	. В
	ATOM	947	N	ARG	138	35.234	9.829	45.135	1.00 22.72	В
	ATOM	948	CA	ARG	138	34.789	8.927	44.075	1.00 22.41	В
	MOTA	949	CB	ARG	138	35.378		44.270	1.00 21.69	В
10	MOTA	950	CG	ARG	138	36.860	7.433	43.951	1.00 20.35	В
	MOTA	951	CD	ARG	138	37.395	6.072	44.347	1.00 17.89	. B
	MOTA	952	NE	ARG	138	38.847	6.020	44.275	1.00 17.83	В
	MOTA	953	CZ	ARG	138	39.529	5.905	43.142		
		954		ARG	138			41.987	1.00 18.07	В
15	MOTA	955		ARG		38.886	5.818 5.906	43.156	1.00 19.38	В
13	MOTA				138 .	40.854			1.00 18.54	В
	ATOM ATOM	956	C	ARG	138	33.263	8.829	44.007	1.00 22.14	В
			. 0	ARG	138	32.689	8.890	42.942	1.00 23.68	В
	MOTA	958	N	THR	139	32.615	8.678	45.154	1.00 22.12	В
20	ATOM	959	CA	THR	139	31.161	8.566	45.203	1.00 25.57	В
20	ATOM	960	CB	THR	139	30.675	8.360	46.662	1.00 25.67	В
	MOTA	961		THR	139	31.355	7.236	47.234	1.00 27.07	В
	ATOM	962		THR	139	29.174	8.100	46.700	1.00 27.35	В
	ATOM	963	c	THR	139	30.463	9.797	44.614	1.00 26.55	В
25	MOTA	964	0	THR	139	29.544	9.675	43.809	1.00 26.69	В
23	ATOM	965	N	LEU	140	30.910	10.982	45.017	1.00 27.11	· B
	MOTA	966	CA	LEU	140	30.314	12.213	44.523	1.00 26.17	В
	MOTA	967		LEU	140	30.949	13.424	45.209	1.00 26.20	В
	MOTA	968	CG	LEU	140	30.599	13.605	46.690	1.00 26.65	В
30	MOTA	969		LEU	140	31.435	14.723	47.280	1.00 25.28	В
30	MOTA	970		LEU	140	29.114	13.896	46.849	1.00 24.93	В
	MOTA	971	C	LEU	140	30.473	12.320	43.018	1.00 25.73	В
	MOTA	972	0	LEU	140	29.556	12.725	42.333	1.00 25.93	· В
	MOTA	973	N	HIS	141	31.641	11.941	42.514	1.00 25.67	В
35	MOTA	974	CA	HIS	141	31.907	12.001	41.081	1.00 26.55	В
33	MOTA	975	CB	HIS	141	33.394	11.743	40.813	1.00 25.96	В
	MOTA	976	CG	HIS	141	33.770	11.804	39.364	1.00 26.57	В
	MOTA	977		HIS	141	33.823	10.841	38.415	1.00 28.59	В
•	MOTA	978		HIS	141	34.138	12.974	38.739	1.00 29.67	В
40	MOTA	979		HIS	141	34.405	12.731	37.467	1.00 29.67	В
40	MOTA	980		HIS	141	34.221	11.443	37.245	1.00 28.28	В
	MOTA	981	C	HIS	141	31.072	10.973	-0.500	1.00 26.86	В
	MOTA	982	0	HIS	141	30.679	11.199	39.181	1.00 28.03	В
	MOTA	983	N	GLN	142	30.802	9.844	40.965	1.00 24.80	В
45	MOTA	984	CA	GLN	142	30.045	8.780	40.326	1.00 25.14	В
43	ATOM	985	CB	GLN	142	30.353	7.436	40.994	1.00 27.48	В
	MOTA	986	CG	GLN	142	31.680	6.834	40.563	1.00 30.52	В
	MOTA	987	CD	GLN	142	31.684	6.417	39.102	1.00 34.29	В
	MOTA	988		GLN	142	30.990	5.475	38.711	1.00 34.96	В
50	MOTA	989		GLN	142	32.468	7.116	38.287	1.00 35.49	В
50	MOTA	990	C	GLN	142	28.550	9.017	40.317	1.00 22.70	В
	MOTA	991	0	GLN	142	27.856	8.528	39.440	1.00 21.46	В
	ATOM	992	N	ILE	143	28.058	9.766	41.297	1.00 21.92	В
	MOTA	993	CA	ILE	143	26.634	10.062	41.365	1.00 22.81	В
55	ATOM	994	CB	ILE	143	26.304	10.888	42.620	1.00 22.20	В
33	ATOM	995		ILE	143	24.880	11.423	42.533	1.00 22.62	В
	ATOM	996			143	26.476	10.024	43.872	1.00 21.94	В
	MOTA	997			143	26.390		45.177		В
	MOTA	998	C	ILE	143	26.187	10.824	40.114	1.00 24.31	В
60	MOTA	999	0	ILE	143	25.156	10.525	39.544	1.00 24.61	В
00	ATOM	1000	N	PHE	144	26.987	11.803	39.693	1.00 26.83	В
	MOTA	1001	CA	PHE	144	26.672	12.611	38.511	1.00 28.06	В
	ATOM	1002	CB	PHE	144	27.580	13.857	38.439	1.00 26.87	В
	MOTA	1003	CG	PHE	144	27.330	14.861	39.536	1.00 27.89	В
65	MOTA	1004		PHE	144	26.169	15.630	39.545	1.00 29.48	В.
U.J	MOTA	1005		PHE	144	28.230	15.002	40.592	1.00 28.77	В
	MOTA	1006		PHE	144	25.901	16.518	40.592	1.00 28.27	В
	ATOM	1007		PHE	144	27.974	15.890	41.647	1.00 28.13	В
	ATOM	1008	CZ	PHE	144	26.805	16.646	41.646	1.00 30.04	В
70	ATOM	1009	C	PHE	144		11.778	37.238	1.00 28.29	В
70	ATOM	1010	0	PHE	144	26.140	12.025	36.253	1.00 28.71	В
	ATOM	1011	N	GLU	145	27.703	10.786	37.273	1.00 29.40	В
	ATOM	1012	CA	GLU	145	27.915	9.909	36.122	1.00 31.01	В
	MOTA	1013	CB	GLU	145	29.216	9.129	36.297	1.00 32.65	В

	MOTA	1014	CG	GLU	145	30.467	9.938	36.056	1.00 38.99	В
	MOTA	1015	CD	GLU	145	30.706	10.197	34.578	1.00 43.44	В
	MOTA	1016		GLU	145	31.623	10.987	34.246	1.00 45.83	В
	MOTA	1017		. GLU	145	29.977	9.603	33.752	1.00 45.50	B
5	ATOM	1018	С	GLU	145	26.753	8.926	35.940	1.00 31.44	В
	MOTA	1019	0	GLU	145	26.237	8.754	34.841	1.00 30.51	В
	ATOM	1020	N	LYS	146	26.348	8.290	37.033	1.00 31.75	В
	ATOM	1021	CA	LYS	146	25.269	7.310	37.012	1.00 33.61	В
	ATOM	1022	CB	LYS	146	25.172		38.381		
10							6.629		1.00 34.03	В
10	ATOM	1023	CG	LYS	146	26.350	5.717	38.695	1.00 38.09	В
	MOTA	1024	, CD	LYS	146	26.243	5.107	40.086	1.00 40.00	В
	MOTA	1025	CE	LYS	146	27.228		40.263	1.00 43.91	В
	ATOM	1026	NZ	LYS	146	26.919	2.818	39.352	1.00 43.76	В
	MOTA	1027	С	LYS	146	23.908	7.882	36.624	1.00 33.97	В
15	ATOM	1028	ō	LYS	146	23.171	7.276	35.840	1.00 33.52	В
	ATOM	1029	N	LEU	147	23.577	9.046	37.176	1:00 33.52	В
	ATOM	1030	CA	LEU	147	22.302	9.689	36.892	1.00 32.92	В
•	MOTA	1031	CB	LEU	147	21.746	10.320	38.175	1.00 31.38	В
ΔΔ.	MOTA	1032	CG	LEU	147	21.336	9.359	39.302	1.00 32.23	В
20	MOTA	1033	CD1	LEU	147	21.060	10.138	40.585	1.00 31.01	В
	ATOM	1034	CD2	LEU	147	20.096	8.569	38.883	1.00 32.23	В
	ATOM	1035	С	LEU	147	22.418	10.749	35.794	1.00 32.85	. 3
	ATOM	1036	ō	LEU	147	21.562	11.609	35.669	1.00 33.29	B .
25	MOTA	1037	N	THR	148	23.475	10.666	34.992	1.00 33.48	.B
23	MOTA	1038	CA	THR	148	23.701	11.636	33.921	1.00 35.96	В
	MOTA	1039	CB	THR	148	24.900	11.236	33.036	1.00 36.22	В
	MOTA	1040	OG1	THR	148	25.074	12.218	32.008	1.00 37.20	В
	MOTA	1041	CG2	THR	148	24:664	9.871	32.381	1.00 38.66	В
	MOTA	1042	С	THR	148	22.484	11.879	33.014	1.00 36.52	. B
30	MOTA	1043	ō	THR	148	22.123	13.021	32.772	1.00 35.06	В
-			-							
	MOTA	1044	N	ASP	149	21.868	10.806	32.514	1.00 35.79	В
	MOTA	1045	CA	ASP	149	20.690	10.923	31.648	1.00 35.29	В
	MOTA	1046	CB	ASP	149	21.101	11.265	30.206	1.00 36.06	В
~~ '	MOTA	1047	CG	ASP	149	22.065	10.249	29.607	1.00 37.80	В
35	ATOM	1048	OD1	ASP	149	22.292	9.196	30.243	1.00 40.41	В
•	ATOM	1049		ASP	149	22.590	10.500	28.496	1.00 36.11	В
•	ATOM	1050	Ċ	ASP	149	19.821	9.657	31.646	1.00 34.60	В
	MOTA	1051	0	ASP	149	19.397	9.184	30.592	1.00 31.15	В
40	MOTA	1052	N	ASN	150	19.554	9.122	32.834	1.00 34.29	В
40	MOTA	1053	CA	.asn	150	18.732	7.923	32.948	1.00 35.52	В
	MOTA	1054	CB	ASN	150	19.227	7.041	34.102	1.00 32.56	В
	ATOM	1055	CG	ASN	150	19.031	7.690	35.452	1.00 32.34	В
	ATOM	1056	OD1	ASN	150	19.134	8.903	35.579	1.00 29.46	В
	ATOM	1057		ASN	150	18.760	6.877	36.475	1.00 31.14	В
45	ATOM	1058	C	ASN	150	17.265	8.292			
13								33.154	1.00 36.96	В
	MOTA	1059	0	ASN	150	16.436	7.431	33.447	1.00 37.74	В
	MOTA	1060	N.	GLY	151	16.953	9.578	32.996	1.00 37.37	В
	MOTA	1061	CA	GLY	151	15.585	10.044	33.153	1.00 37.75	В
	MOTA	1062	С	GLY	151	15.195	10.351	34.585	1.00 39.12	В
50	MOTA	1063	0	GLY	151	14.013	10.490	34.903	1.00 39.41	В
	ATOM	1064	N	THR	. 152	16.190	10.455	35.455	1.00 40.74	В
	ATOM	1065	CA	THR	152	15.950	10.748	36.860	1.00 42.40	В
	ATOM	1066	СВ	THR	152	16.587	9.674	37.772		
									1.00 42.88	В
55	ATOM	1067		THR	152	16.143	8.375	37.365	1.00 46.42	В
22	MOTA	1068	CG2	THR	152	16.182	9.891	39.221	1.00 43.02	В
	MOTA	1069	C	THR	152	16.537	12.108	37.216	1.00 42.92	В
	MOTA	1070	0	THR	152	17.753	12.303	37.176	1.00 45.15	В
	MOTA	1071	N	GLU	153	15.657	13.050	37.539	1.00 41.16	В
	MOTA	1072	CA	GLU	153	16.083	14.390	37.910	1.00 39.15	В
60 -	ATOM	1073	CB	GLU	153		15.350			
00						14.902		37.865	1.00 41.46	В
	MOTA	1074	CG	GLU	153	15.290	16.742	37.456	1.00 46.88	В
	MOTA	1075	CD	GLU	153	15.645	16.826	35.983	1.00 50.26	В
	ATOM	1076	0E1	GLU	153	16.309	17.808	35.591	1.00 54.28	В
	MOTA	1077	OE2		153	15.256	15.920	35.216	1.00 50.49	В
65	ATOM	1078	C	GLU	153		14.273	39.336	1.00 35.77	В
	MOTA	1079	ŏ	GLU	153	16.024	13.550	40.143	1.00 34.39	
										В
	MOTA	1080	N	PHE	154	17.676	14.986	39.649	1.00 32.19	В
	MOTA	1081	CA	PHE	154	18.247	14.903	40.985	1.00 29.64	B
70	MOTA	1082	CB	PHE	154	19.221	13.731	41.036	1.00 26.07	В
70	MOTA	1083	CG	PHE	154	20.478	13.959	40.244	1.00 22.24	В
	MOTA	1084	CD1		154	21.634	14.413	40.870	1.00 19.12	В
	ATOM	1085	CD2		154	20.502	13.725	38.873	1.00 19.79	В
	ATOM	1086	CEI		154	22.804	14.627		1.00 19.79	
		1000			194 .	22.004	14.02/	40.140	1.00 20.1/	В

	MOTA	1087		PHE	154	21.665	13.938	38.132	1.00 19.68	В
	MOTA	1088	CZ	PHE	154	22.819	14.388	38.768	1.00 18.22	В
	ATOM ATOM	1089 1090	0	PHE	154 154	18.983 19.343	16.153	41.462	1.00 28.59 1.00 28.03	B B
5	ATOM	1091	N	SER	155	19.219	16.194	42.765	1.00 28.62	В
	ATOM	1092	CA	SER	155	19.940	17.286	43.398	1.00 29.65	В
	MOTA	1093	CB	SER	155	18.958	18.297	44.007	1.00 29.30	В
	MOTA	1094	OG	SER	155	18.373	17.825	45.210	1.00 30.25	В
10	MOTA	1095	C	SER	155	20.812		44.495	1.00 29.32	В
10	ATOM ATOM	1096 1097	N N	SER VAL	155 156	20.364 22.057	15.799 17.117	45.236 44.601	1.00 28.78 1.00 28.25	. B
	ATOM	1098	CA	VAL	156	22.945	16.571	45.622	1.00 27.65	. в В
	ATOM	1099	СВ	VAL	156	24.266	16.059	45.002	1.00 27.82	В
1.5	ATOM	1100		VAL	156	25.067	15.296	46.051	1.00 26.25	В
15	MOTA	1101		VAL	156	23.970	15.178	43.793	1.00 26.92	В
	MOTA	1102	c	VAL	156	23.293	17.600	46.697	1.00 28.00	В
	ATOM ATOM	1103 1104	O N	VAL LYS	156 157	23.691 23.135	18.705 17.210	46.386 47.961	1.00 27.61 1.00 28.26	· B B
	ATOM	1105	CA	LYS	157	23.455	18.066	49.107	1.00 29.25	8
20	MOTA	1106	CB	LYS	157	22.188	18.423	49.897	1.00 30.98	В
	MOTA	1107	CG	LYS	157	21.322	19.485	49.261	1.00 34.09	В
	ATOM	1108	CD	LYS	157	20.065	19.741	50.080	1.00 37.95	В
	MOTA MOTA	1109 1110	CE NZ	LYS	157 157	19.399 20.186	21.060 22.277	49.665	1.00 41.02	В
25	ATOM	1111	C	LYS	157	24.426	17.349	50.077 50.047	1.00 41.43	B
	ATOM	1112	ŏ	LYS	157	24.195	16.217	50.413	1.00 28.14	В
	MOTA	1113	N	, VAL	158	25.510	18.016	50.433	1.00 27.07	В
	MOTA	1114	CA	VAL	158	26.480	17.412	51.342	1.00 27.48	В
30	MOTA	1115	CB	VAL	158	27.883	17.280	50.694	1.00 26.91	В
50	MOTA MOTA	1116 1117		VAL VAL	158 158	27.811 28.415	16.356 18.648	49.489 50.301	1.00 27.77 1.00 27.25	B B
	ATOM	1118	C	VAL	158	26.629	18.183	52.651	1.00 27.25	В
	MOTA	1119	0	VAL	158	26.444	19.393	52.705	1.00 27.69	B
25	MOTA	1120	N	SER	159	26.973	17.460	53.708	1.00 28.98	В
35	ATOM	1121	CA	SER	159	27.155	18.058	55.013	1.00 30.95	В.
	MOTA MOTA	1122 1123	CB OG	SER	159	25.869	17.953	55.823	1.00 32.26	В
	ATOM	1123	C	SER SER	159 159	24.817 28.289	18.602 17.362	55.132 55.736	1.00 38.42 1.00 30.96	B B
	ATOM	1125	ŏ	SER	159	28.388	16.146	55.722	1.00 34.27	В
40	MOTA	1126	N	LEU	160	29.158	18.143	56.357	1.00 29.31	В
	MOTA	1127	CA	LEU	160	30.280	17.577	57.064	1.00 27.33	В
	MOTA	1128	CB	LEU	160	31.582	18.130	56.499	1.00 27.18	В
	ATOM ATOM	1129 1130	CG CD1	LEU	160 160	32.856 32.751	17.456 15.954	56.991 56.790	1.00 28.13 1.00 29.56	B B
45	ATOM	1131		LEU	160	34.044	18.019	56.237	1.00 28.17	В
	MOTA	1132	С	LEU	160	30.167	17.884	58.552	1.00 28.09	В
	ATOM	1133	0	LEU	160	30.607	18.943	59.026	1.00 26.39	В
	MOTA	1134	N	LEU	161	29.558	16.949	59.276	1.00 25.48	В
50	MOTA MOTA	1135 1136	CA CB	LEU LEU	161 161	29.371 27.982	17.075 16.567	60.710 61.101	1.00 23.19 1.00 21.33	B B
-	ATOM	1137	CG	LEU	161	27.694	16.395	62.594	1.00 19.50	B
	ATOM	1138		LEU	161	27.772	17.736	63.288	1.00 19.94	В
	MOTA	1139		LEU	161	26.314	15.775	62.782	1.00 17.88	В
55	MOTA	1140	C	LEU	161	30.452	16.264	61.415	1.00 23.39	В
33	ATOM ATOM	1141 1142	N O	LEU GLU	161 162	30.641 31.165	15.094 16.899	61.129 62.336	1.00 25.56 1.00 22.32	B B
	ATOM		CA	GLU	162	32.232		63.065		В
	MOTA	1144	CB	GLU	162	33.574	16.839	62.650	1.00 17.28	В
60	MOTA	1145	CG	GLU	162	33.762	16.859	61.137	1.00 15.11	В
60	MOTA	1146	CD	GLU	162	35.212	16.937	60.737	1.00 15.23	В
	MOTA MOTA	1147 1148		GLU	162 162	36.063	17.134	61.621	1.00 15.82	В
	ATOM	1149	C	GLU	162	35.513 32.031	16.813 16.344	59.539 64.573	1.00 17.71 1.00 19.72	B B
	ATOM	1150	ō	GLU	162	31.468	17.299	65.059	1.00 20.94	В
65	MOTA	1151	N	ILE	163	32.503	15.348	65.312	1.00 18.63	В
	MOTA	1152	CA	ILE	163	32.346	15.350	66.756	1.00 18.63	В
	ATOM	1153	CB	ILE	163	31.544	14.120	67.223	1.00 19.02	В
	MOTA MOTA	1154		ILE	163	31.324	14.178	68.742	1.00 16.34	В
70	MOTA	1155 1156		ILE	163 163	30.210 29.479	14.072 12.746	66.466 66.563	1.00 20.01 1.00 22.19	B B
	MOTA	1157	C	ILE	163	33.694	15.353	67.467	1.00 20.32	В
	MOTA	1158	0	ILE	163	34.616	14.672	67.050	1.00 21.59	В
	MOTA	1159	N	TYR	164	33.799	16.131	68.542	1.00 20.27	В

	MOTA	1160	CA	TYR	164		35.031	16.206	69.312	1.00 19.83	В
	ATOM	1161	CB	TYR	164		35.964	17.271	68.709		
										1.00 20.10	
	ATOM	1162	CG	TYR	164		37.269	17.434	69.451	1.00 17.1	_
_	MOTA	1163	CD1	TYR	164		37.334	18.191	70.622	1.00 16.03	3 B
5	ATOM	1164	CE1	TYR	164		38.506	18.253	71.372	1.00 16.71	l B
	MOTA	1165	CD2	TYR	164		38.416	16.756	69.042	1.00 18.6	7 B
	MOTA	1166	CE2		164		39.594	16.812	69.789	1.00 16.74	
	MOTA	1167	CZ	TYR	164		39.627	17.557	70.954		
•										1.00 14.83	
10	MOTA	1168	ОН	TYR	164		40.758	17.569	71.726	1.00 14.9	
10	MOTA	1169	С	TYR	164		34.685	16.520	70.761	1.00 21.32	2 B
	MOTA -	1170	.0	TYR	164		33.971	17.468	71.044	1.00 22.73	L B
	MOTA	1171	N	ASN	165		35.185	15.694	71.672	1.00 22.32	2 в
	MOTA	1172	CA	ASN	165		34.926	15.860	73.092	1.00 23.78	
	ATOM	1173	СВ	ASN	165		35.722	17.043	73.636	1.00 27.16	
15	MOTA	1174									
IJ			CG	ASN	165		35.729	17.090	75.149	1.00 31.99	
	MOTA	1175		ASN	165		36.159	16.150	75.801	1.00 37.27	
	MOTA	1176	ND2	asn	165		35.249	18.190	75.714	1.00 32.43	В В
	MOTA	1177	С	ASN	165		33.431	16.088	73.313	1.00 24.23	3 в
	ATOM	1178	0	ASN	165		33.034	16.915	74.130	1.00 25.34	В
20	ATOM	1179	N	GLU	166		32.615	15.340	72.572	1.00 22.3	
	ATOM	1180	CA	GLU	166		31.154	15.421	72.641		
										1.00 22.51	
	ATOM	1181	СВ	GLU	166		30.638	15.047	74.044	1.00 19.36	
	MOTA	1182	CG	GLU	166		30.620	13.540	74.319	1.00 20.22	
25	MOTA	1183	CD	GLU	166		29.915	12.746	73.222	1.00 20.03	L ∂B
25	MOTA	1184	OE1	GLU	166		28.668	12.648	73.240	1.00 19.99	Э В
	MOTA	1185	OE2	GLU	166		30.618	12.228	72.330	1.00 16.49	
	ATOM	1186	C	GLU	166		30.570	16.770	72.223	1.00 22.98	
	ATOM	1187	ŏ	GLU	166		29:553	17.189	72.725	1.00 22.40	
						•					
30	ATOM	1188	N	GLU	167		31.229	17.443	71.288	1.00 25.41	
30	MOTA	1189	CA	GLU	167		30.739	18.721	70.793	1.00 27.30	
	MOTA	1190	CB	GLU	167		31.679	19.858	71.191	1.00 29.98	3 B
	ATOM	1191	CG	GLU	167		31.567	20.295	72.648	1.00 34.85	5 B
	ATOM	1192	CD	GLU	167		32.384	21.553	72.941	1.00 39.75	5 В
	MOTA	1193		GLU	167		33.635	21.487	72.865	1.00 39.56	
35·	ATOM	.1194	OE2		167		31.771	22.608	73.237	1.00 41.26	
55											
•	MOTA	1195	C	GLU	167		30.637	18.626	69.278	1.00 28.54	
	MOTA	1196	0	GLU	167		31.495	18.046	68.633	1.00 29.56	5 В
	MOTA	1197	N	LEU	168		29.574	19.190	68.719	1.00 28.34	В
	MOTA	1198	CA	LEU	168		29.367	19.138	67.280	1.00 28.28	3 В
40	MOTA	1199	CB	LEU	168		27.865	19.078	66.955	1.00 30.49	
	ATOM	1200	CG	LEU	168		27.009	17.925	67.512	1.00 30.82	
	ATOM	1201		LEU	168		27.623	16.583	67.142		
										1.00 31.07	
	ATOM	1202		LEU	168		26.892	18.044	69.009	1.00 33.15	
15	MOTA	1203	C	LEU	168		29.997	20.322	66.563	1.00 26.93	
45	MOTA	1204	0	LEU	168		29.972	21.442	67.064	1.00 28.48	3 в
	MOTA	1205	N	PHE	169		30.562	20.069	65.386	1.00 24.01	L. B
	MOTA	1206	CA	PHE	169		31.191	21.112	64.584	1.00 22.58	3 B
	ATOM	1207	CB	PHE	169	•	32.723	21.073	64.727	1.00 22.71	
	ATOM	1208	CG	PHE	169		33.213	21.377	66.118	1.00 21.76	
50											
50	MOTA	1209		PHE	169		33.451	20.354	67.027	1.00 21.14	
	MOTA	1210		PHE	169		33.393	22.699	66.534	1.00 22.60	
	MOTA	1211		PHE	169		33.861	20.628	68.323	1.00 22.05	
	MOTA	1212	CE2	PHE	169		33.802	22.989	67.830	1.00 21.62	
	MOTA	1213	CZ	PHE	169		34.037	21.952	68.729	1.00 24.67	7 B
55	MOTA	1214	С	PHE	169		30.824	20.950	63.111	1.00 23.10	
	MOTA	1215	Ō	PHE	169		30.612	19.836	62.634	1.00 20.06	
	ATOM	1216	N	ASP	170		30.739	22.079	62.406	1.00 22.96	
		1217									
	MOTA		CA	ASP	170		30.416	22.100	60.978	1.00 22.20	
۲۸	MOTA	1218	CB	ASP	170		29.344	23.148	60.679	1.00 20.54	
60	ATOM	1219	CG	ASP	170		28.799	23.048	59.257	1.00 21.66	5 В
	MOTA	1220	OD1	ASP	170		29.554	22.671	58.337	1.00 18.77	7 B
	MOTA	1221	OD2	ASP	170		27.602	23.358	59.065	1.00 23.66	5 B
	ATOM	1222	C	ASP	170		31.680	22.466	60.211	1.00 22.85	
	ATOM	1223	ŏ	ASP	170		32.108	23.621	60.242	1.00 25.36	
65											_
0,5	MOTA	1224	N	LEU	171		32.280	21.490	59.529	1.00 22.35	
	MOTA	1225	CA	LEU	171		33.494	21.729	58.764	1.00 22.58	
	MOTA	1226	CB	LEU	171		34.430	20.533	58.864	1.00 16.27	7 В
	MOTA	1227	CG	LEU	171		35.235	20.424	60.169	1.00 16.39	
	MOTA	1228		LEU	171		36.234	21.577	60.274	1.00 14.32	
70	ATOM	1229		LEU	171		34.304	20.421	61.351	1.00 12.71	
	MOTA	1230	C	LEU	171		33.257	22.082	57.300	1.00 26.58	
	ATOM	1231	0	LEU	171		34.167	21.976	56.479	1.00 26.75	
	MOTA	1232	N	LEU	172		32.038	22.510	56.978	1.00 29.45	5 B

ATOM 1233 CA LEU 172 31.706 22.898 ATOM 1234 CB LEU 172 30.742 21.892 ATOM 1235 CG LEU 172 31.387 20.715 ATOM 1236 CD1 LEU 172 30.316 19.992 5 ATOM 1237 CD2 LEU 172 32.473 21.201 ATOM 1238 C LEU 172 32.473 21.201 ATOM 1239 O LEU 172 30.961 24.850 ATOM 1240 N ASN 173 30.766 24.865	55.612 1.00 34.57 B 54.975 1.00 33.36 B 54.244 1.00 31.35 B 53.459 1.00 32.85 B 53.302 1.00 32.08 B 55.531 1.00 38.00 B
ATOM 1234 CB LEU 172 30.742 21.892 ATOM 1235 CG LEU 172 31.387 20.715 ATOM 1236 CD1 LEU 172 30.316 19.992 ATOM 1237 CD2 LEU 172 32.473 21.201 ATOM 1238 C LEU 172 31.107 24.297 ATOM 1239 0 LEU 172 30.961 24.850	54.975 1.00 33.36 B 54.244 1.00 31.35 B 53.459 1.00 32.85 B 53.302 1.00 32.08 B
ATOM 1235 CG LEU 172 31.387 20.715 ATOM 1236 CD1 LEU 172 30.316 19.992 5 ATOM 1237 CD2 LEU 172 32.473 21.201 ATOM 1238 C LEU 172 31.107 24.297 ATOM 1239 0 LEU 172 30.961 24.850	54.244 1.00 31.35 B 53.459 1.00 32.85 B 53.302 1.00 32.08 B
5 ATOM 1236 CD1 LEU 172 30.316 19.992 ATOM 1237 CD2 LEU 172 32.473 21.201 ATOM 1238 C LEU 172 31.107 24.297 ATOM 1239 O LEU 172 30.961 24.850	53.459 1.00 32.85 B 53.302 1.00 32.08 B
5 ATOM 1237 CD2 LEU 172 32.473 21.201 ATOM 1238 C LEU 172 31.107 24.297 ATOM 1239 O LEU 172 30.961 24.850	53.302 1.00 32.08 B
ATOM 1238 C LEU 172 31.107 24.297 ATOM 1239 O LEU 172 30.961 24.850	
ATOM 1239 O LEU 172 30.961 24.850	JJ.JJ1 1.00 JU.00 B
	54.457 1.00 39.59 B
10 ATOM 1241 CA ASN 173 30.201 26.205 ATOM 1242 CB ASN 173 29.401 26.405	56.714 1.00 45.99 B
	58.003 1.00 47.65 B
ATOM 1243 CG ASN 173 28.670 27.735	58.038 1.00 50.77 B
ATOM 1244 OD1 ASN 173 28.005 28.060	59.014 1.00 51.85 B
ATOM 1245 ND2 ASN 173 28.792 28.508	56.964 1.00 51.20 B
ATOM 1246 C ASN 173 31.346 27.214	56.643 1.00 48.84 B
15 ATOM 1247 O ASN 173 . 32.070 27.403	57.606 1.00 48.46 B
ATOM 1248 N PRO 174 . 31.521 27.872	55.484 1.00 52.47 B
ATOM 1249 CD PRO 174 30.710 27.738	54.258 1.00 53.23 B
ATOM 1250 CA PRO 174 32.587 28.862	55.289 1.00 55.00 B
ATOM 1251 CB PRO 174 32.542 29.116	53.786 1.00 53.92 B
20 ATOM 1252 CG PRO 174 31.089 28.983	53.482 1.00 52.93 B
ATOM 1253 C PRO 174 32.396 30.141	56.095 1.00 58.07 B
ATOM 1254 O PRO 174 33.329 30.921	56.263 1.00 58.84 B
ATOM 1255 N SER 175 31.183 30.343	56.596 1.00 60.39 B
ATOM 1256 CA SER 175 30 861 31 534	57.372 1.00 62.65 B
25 ATOM 1257 CB SER 175 29.343 31.666	57.498 1.00 63.30 B
ATOM 1258 OG SER 175 28.723 31.545	56.230 1.00 65.14 B
ATOM 1259 C SER 175 31.500 31.535	58.759 1.00 63.89 B
ATOM 1260 O SER 175 32.365 32.358	59.051 1.00 65.71 B
ATOM 1261 N SER 176 31.066 30.608	59.608 1.00 64.41 B
30 ATOM 1262 CA SER 176 31.581 30.506	60.969 1.00 64.51 B
ATOM 1263 CB SER 176 30.597 29.725	61.844 1.00 64.33 B
ATOM 1264 OG SER 176 30.446 28.396	
ATOM 1265 C SER 176 30.446 28.396	61.378 1.00 64.08 B 61.012 1.00 64.78 B
	62.213 1.00 65.17 B
ATOM 1268 CA ASP 177 34.789 29.051	62.379 1.00 65.62 B
ATOM 1269 CB ASP 177 35.782 29.964	63.106 1.00 66.73 B
ATOM 1270 CG ASP 177 35.449 30.137	64.576 1.00 68.48 B
ATOM 1271 OD1 ASP 177 36.388 30.344	65.377 1.00 67.76 B
40 ATOM 1272 OD2 ASP 177 34.251 30.069	64.929 1.00 69.81 B
ATOM 1273 C ASP 177 34.615 27.757	63.166 1.00 64.60 B
ATOM 1274 O ASP 177 33.498 27.335	63.445 1.00 64.22 B
ATOM 1275 N VAL 178 35.737 27.146	63.529 1.00 63.40 B
ATOM 1276 CA VAL 178 35.735 25.890	64.264 1.00 62.69 B
45 ATOM 1277 CB VAL 178 37.046 25.116	64.016 1.00 62.85 B
ATOM 1278 CG1 VAL 178 37.190 24.809	62.536 1.00 61.71 B
ATOM 1279 CG2 VAL 178 38.231 25.934	64.510 1.00 62.99 B
ATOM 1280 C VAL 178 35.552 26.050	65.770 1.00 61.94 B
ATOM 1281 O VAL 178 35.792 25.122	66.524 1.00 62.60 B
50 ATOM 1282 N SER 179 35.124 27.227	66.208 1.00 61.07 B
ATOM 1283 CA SER 179 34.922 27.447	67.632 1.00 59.46 B
ATOM 1284 CB SER 179 35.629 28.731	68.080 1.00 59.42 B
ATOM 1285 OG SER 179 35.030 29.877	67.507 1.00 59.13 B
ATOM 1286 C SER 179 33 437 27 517	67.977 1.00 58.68 B
55 ATOM 1287 O SER 179 33.067 27.489	69.144 1.00 59.17 B
ATOM 1288 N GLU 180 32.591 27.605	66.955 1.00 56.65 B
ATOM 1289 CA GLU 180 31.145 27.671	67.161 1.00 55.22 B
ATOM 1290 CB GLU 180 30.507 28.607	66.129 1.00 56.66 B
ATOM 1291 CG GLU 180 30.550 30.079	66.535 1.00 59.12 B
60 ATOM 1292 CD GLU 180 30.230 31.032	65.392 1.00 60.03 B
ATOM 1293 OE1 GLU 180 31.066 31.163	64.474 1.00 60.45 B
ATOM 1294 OE2 GLU 180 29.143 31.650	65.411 1.00 61.47 B
ATOM 1295 C GLU 180 30.498 26.293 ATOM 1296 O GLU 180 30.207 25.803	67.080 1.00 52.95 B
	66.004 1.00 52 86 B
	68.239 1.00 51.12 B
ATOM 1298 CA ARG 181 29.675 24.360	68.315 1.00 48.73 B
ATOM 1299 CB ARG 181 29.835 23.793	69.727 1.00 51.62 B
	70.836 1.00 56.45 B
ATOM 1300 CG ARG 181 29.642 24.816	77 HA7 1 AN 61 66 P
ATOM 1301 CD ARG 181 28.829 24.256	72.007 1.00 61.65 B
70 ATOM 1301 CD ARG 181 28.829 24.256 ATOM 1302 NE ARG 181 27.400 24.135	71.702 1.00 64.33 B
70 ATOM 1301 CD ARG 181 28.829 24.256 ATOM 1302 NE ARG 181 27.400 24.135 ATOM 1303 CZ ARG 181 26.483 23.692	71.702 1.00 64.33 B 72.560 1.00 65.71 B
70 ATOM 1301 CD ARG 181 28.829 24.256 ATOM 1302 NE ARG 181 27.400 24.135	71.702 1.00 64.33 B

	MOTA	1306	С	ARG	181	28.196	24.403	67.940	1.00 45.46	В
	MOTA	1307	ŏ	ARG	181	27.556	25.438	68.029	1.00 45.33	В
	MOTA	1308	N	LEU	182	27.661	23.267	67.510	1.00 41.98	B
	MOTA	1309	CA	LEU	182	26.258	23.193	67.133	1.00 38.04	В
5	MOTA	1310	CB	LEU	182	26.099	22.419	65.824	1.00 35.02	В
	MOTA	1311	CG	LEU	182	26.990	22.896	64.677	1.00 33.00	В
	MOTA	1312		LEU	182	26.723	22.060	63.450	1.00 31.57	В
	ATOM	1313		Leu	182	26.733	24.372	64.393	1.00 32.49	В
10	MOTA	1314	C	LEU	182	25.456	22.524	68.236	1.00 38.00	В
10	MOTA	1315	0	LEU	182	26.017	21.845	69.096	1.00 37.75	В
	MOTA	1316	N	GLN	183	24.140	22.723	68.206	1.00 37.43 1.00 36.96	В
	MOTA MOTA	1317 1318	CA CB	GLN GLN	183 183	23.239 22.269	22.148 23.210	69.200 69.724	1.00 38.87	B B
•	MOTA	1319	CG	GLN	183	22.925	24.543	70.024	1.00 43.04	В
15	MOTA	1320	CD	GLN	183	21.969	25.536	70.653	1.00 45.13	В
	ATOM	1321		GLN	183	21.663	25.448	71.832	1.00 45.23	B
	ATOM	1322	NE2		183	21.493	26.492	69.856	1.00 46.40	В
	MOTA	1323	С	GLN	183	22.455	21.018	68.567	1.00 35.80	В
20	MOTA	1324	0	GLN	183	22.097	21.073	67.397	1.00 33.40	В
20	MOTA	1325	N	MET	184	22.165	20.005	69.367	1.00 36.43	. В
	MOTA	1326	CA	MET	184	21.450	18.840	68.877	1.00 37.65	В
	MOTA	1327	CB	MET	184	22.322	17.610	69.118	1.00 38.53	В.
	MOTA	1328 1329	CG	MET MET	184	22.033	16.445	68.221	1.00 41.45	В
25	MOTA MOTA	1330	SD	MET	184 184	23.141 22.590	15.085 14.660	68.586 70.190	1.00 42.59 1.00 40.16	·B B
23	MOTA	1331	C	MET	184	20.111	18.692	69.590	1.00 40.16	8
	ATOM	1332	ŏ	MET	184	20.021	18.909	70.790	1.00 37.22	B
	ATOM	1333	N	PHE	185	. 19:070	18.328	68.844	1.00 39.01	. в
	MOTA	1334	CA	PHE	185	17.741	18.148	69.432	1.00 41.26	В
30	MOTA	1335	CB	PHE	185	16.851	19.377	69.160	1.00 40.10	В
	MOTA	1336	CG	PHE	185	17.499	20.697	69.494	1.00 38.50	В
	ATOM	1337		PHE	185	18.249	21.377	68.544	1.00 36.52	В
	ATOM	1338		PHE	185	17.376	21.248	70.770	1.00 38.29	В
35 ·	ATOM	1339		PHE	185	18.869	22.586	68.851	1.00 37.06	В
23	MOTA MOTA	·1340 1341		PHE	185 185	17.994 18.743	22.459	71.089	1.00 37.60	В
•	MOTA	1342	CZ C	PHE	185	17.034	23.128 16.903	70.128 68.887	1.00 37.41 1.00 43.21	B B
	MOTA	1343	ŏ	PHE	185	17.221	16.532	67.734	1.00 41.62	В
	ATOM	1344	N	ASP	186	16.223	16.259	69.724	1.00 46.68	В
40	MOTA	1345	CA	ASP	186	15.482	15.078	69.286	1.00 51.00	В
	MOTA	1346	CB	ASP	186	14.722	14.437	70.449	1.00 52.32	В
	MOTA	1347	CG	ASP	186	15.642	13.912	71.530	1.00 54.63	В
	MOTA	1348		ASP	186	16.575	13.150	71.202	1.00 55.59	В
45	MOTA	1349		ASP	186	15.428	14.262	72.712	1.00 56.98	В
43	MOTA	1350	C	ASP	186	14.481	15.539	68.241	1.00 52.48	В
	MOTA MOTA	1351 1352	0	ASP ASP	186 187	13.777 14.425	16.510	68.443	1.00 52.99	В
	ATOM	1353	N . CA	ASP	187	13.500	14.841 15.214	67.118 66.061	1.00 55.70 1.00 59.24	B B
	MOTA	1354	CB	ASP	187	13.845	14.469	64.772	1.00 58.33	В
50	ATOM	1355	CG	ASP	187	13.015	14.929	63.601	1.00 58.32	В
	ATOM	1356		ASP	187	13.345	14.546	62.459	1.00 59.29	В
	MOTA	1357	OD2	ASP	187	12.035	15.672	63.822	1.00 58.82	В
	MOTA	1358	С	ASP	187	12.064	14.905	66.473	1.00 61.85	В
55	MOTA	1359	0	ASP	187	11.690	13.750	66.626	1.00 62.59	В
33	MOTA	1360	N	PRO	188	11.241	15.950	66.662	1.00 64.18	В
	ATOM	1361	CD	PRO	188	11.573	17.374	66.493	1.00 64.61	В
	ATOM ATOM	1362 1363	CA CB	PRO PRO	188 188	9.840 9.287	15.794 17.207	67.061 66.923	1.00 66.06 1.00 65.95	В
	ATOM	1364	CG	PRO	188	10.472	18.048	67.271	1.00 65.81	B B
60 ·	ATOM	1365	c	PRO	188	9.094	14.793	66.189	1.00 68.16	В
	ATOM	1366	ŏ	PRO	188	8.316	13.981	66.687	1.00 67.45	B
	MOTA	1367	N	ARG	189	9.345	14.854	64.886	1.00 70.27	В
	MOTA	1368	CA	ARG	189	8.702	13.949	63.944	1.00 73.47	В
<i>C</i>	MOTA	1369	CB	ARG	189	9.278	14.170	62.547	1.00 73.94	В
65	MOTA	1370	CG	ARG	189		15.498	61.926	1.00 75.92	В
	MOTA	1371	CD	ARG	189	9.507	15.693	60.558	1.00 77.54	В
	MOTA	1372	NE	ARG	189	10.797	16.373	60.644	1.00 78.29	В
	MOTA	1373	CZ	ARG	189	10.940	17.686	60.804	1.00 78.57	В
70	MOTA MOTA	1374 1375		ARG ARG	189	9.870	18.466	60.894	1.00 78.77	В
/-	MOTA	1376	C NH2	ARG	189 189	12.153 8.869	18.218 12.491	60.873 64.363	1.00 78.05 1.00 75.30	B B
	ATOM	1377	ο.	ARG	189	7.896	11.815	64.683	1.00 75.56	В
	ATOM	1378	N .	ASN	190	10.112	12.019	64.370	1.00 77.42	В

	2001	1220	~		100	10 417	20 640	C4 340	1 00 70 60	_
	ATOM ATOM	1379 1380	CA CB	ASN ASN	190 190	10.417 10.760	10.640 9.829	64.748	1.00 78.69 1.00 78.94	В
	ATOM	1381	CG	ASN	190	11.569	10.629	63.494 62.483	1.00 78.94	B B
	ATOM	1382	OD1		190	12.745	10.025	62.689	1.00 78.51	В
5	ATOM	1383	ND2		190	10.926	11.011	61.383	1.00 78.16	В
	MOTA	1384	C	ASN	190	11.571	10.575	65.749	1.00 79.40	В
	MOTA	1385	0	ASN	190	12.706	10.875	65.408	1.00 79.98	В
	MOTA	1386	N	LYS	191	11.265	10.182	66.986	1.00 79.97	В
10	ATOM	1387	CA	LYS	191	12.267		68.051	1.00 79.77	В
10	MOTA	1388	СВ	LYS	191	11.616	9.561	69.336	1.00 81.11	В
	MOTA	1389	CG	LYS	191	10.794	10.600	70.090	1.00 82.60	• В
	MOTA	1390	CD	LYS	191	11.695	11.630	70.758	1.00 83.37	В
	MOTA MOTA	1391	CE	LYS	191	10.887	12.716	71.450	1.00 84.12	В
15	MOTA	1392 1393	NZ C	LYS LYS	191 191	10.109 13.478	13.539 9.216	70.478 67.695	1.00 84.72 1.00 78.46	В
13	MOTA	1394	ò	LYS	191	14.462	9.173	68.434	1.00 78.48	B B
	ATOM	1395		ARG	192	13.398	8.525	66.563	1.00 76.93	B
	ATOM	1396	CA	ARG	192	14.489	7.675	66.106	1.00 75.17	В
	MOTA	1397	СВ	ARG	192	13.975	6.667	65.078	1.00 77.95	В
20	MOTA	1398	CG	ARG	192	15.041	5.708	64.573	1.00 80.81	В
	ATOM	1399	CD	ARG	192	. 14.801	5.305	63.122	1.00 83.98	В
	ATOM .	1400	NE	ARG	192	14.928	6.434	62.198	1.00 86.03	В
	ATOM	1401	CZ	ARG	192	13.946	7.277	61.884	1.00 86.70	В
25	MOTA	1402		ARG	192	12.737	7.133	62.415	1.00 86.57	В
25	MOTA	1403	NH2		192	14.175	8.267	61.033	1.00 87.03	В
	ATOM ATOM	1404 1405	С 0	ARG ARG	192 192	15.565 16.699	8.545 8.112	65.463		. В
	MOTA	1406	N	GLY	193	15.195	9.781	65.272 65.136	1.00 72.31 1.00 69.32	B B
	ATOM	1407	CA	GLY	193	16.132	10.695	64.507	1.00 63.90	В
30	ATOM	1408	C	GLY	193	16.538	11.863	65.382	1.00 59.50	В
	ATOM	1409	Ō	GLY	193	16.132	11.961	66.531	1.00 59.54	В
	ATOM	1410	N	VAL	194	17.346	12.757	64.824	1.00 55.13	В
	ATOM	1411	CA	VAL	194	17.812	13.918	65.562	1.00 50.91	В
25	ATOM	1412	CB	VAL	194	19.114	13.606	66.309	1.00 50.28	В
35	ATOM	1413		VAL	194	20.226	13.319	65.318	1.00 49.18	В .
	ATOM	1414		VAL	194	19.476	14.760	67.207	1.00 48.67	В
	MOTA MOTA	1415	C	VAL	194	18.055	15.098	64.629	1.00 49.13	В
	ATOM	1416 1417	O N	VAL	194 195	18.379 17:906	14.918 16.308	63.461 65.160	1.00 49.22	В
40	ATOM	1418	CA	ILE	195	18.106	17.514	64.372	1.00 46.55 1.00 42.49	B B
	MOTA	1419	CB	ILE	195	16.846	18.405	64.396	1.00 42.49	В
	MOTA	1420		ILE	195	17.076	19.653	63.561	1.00 44.86	В
	ATOM	1421		ILE	195	15.647	17.639	63.837	1.00 44.25	В
	MOTA	1422	CD1	ILE	195	15.828	17.184	62.393	1.00 45.64	B
45	MOTA	1423	С	ILE	195	19.291	18.349	64.856	1.00 39.72	В
	MOTA	1424	0	ILE	195	19.379	18.691	66.030	1.00 38.69	В
	MOTA	1425	N	ILE	196	20.197	18.672	63.936	1.00 37.40	В
	MOTA	1426	CA	ILE	196	21.365	19.483	64.255	1.00 35.21	В
50	MOTA	1427	CB	ILE	196	22.654	18.960	63.561	1.00 34.42	В
50	ATOM ATOM	1428 1429		ILE	196 196	23.821 23.010	19.880 17.552	63.881 64.057	1.00 33.62	B B
	MOTA	1430		ILE	196	22.222	16.445	63.416	1.00 33.50 1.00 31.23	В
	ATOM	1431	Ç	ILE	196	21.113	20.920	63.806	1.00 35.34	В
	ATOM	1432	ŏ	ILE	196	21.108	21.218	62.619	1.00 33.58	В
55	MOTA	1433	N	LYS	197	20.912	21.806	64.777	1.00 36.02	В
	ATOM	1434	CA	LYS	197	20.639	23.209	64.494	1.00 36.95	В
	MOTA	1435	CB	LYS	197	20.101	23.909	65.744	1.00 37.83	В
	ATOM	1436	CG	LYS	197	19.736	25.370	65.519	1.00 42.01	В
60	ATOM	1437	CD	LYS	197	19.391	26.055	66.829	1.00 45.50	В
UU	MOTA	1438	CE	LYS	197	19.039	27.518	66.628	1.00 46.65	В
	ATOM	1439	NZ	LYS	197	18.686	28.161	67.932	1.00 47.32	В
	MOTA MOTA	1440 1441	С 0	LYS LYS	197 197	21.857	23.968	63.983	1.00 36.01	В
	MOTA	1442	N	GLY	198	22.887 21.722	24.025 24.547	64.646 62.793	1.00 34.47 1.00 35.82	. B
65	ATOM	1443	CA	GLY	198	22.809	25.316	62.212	1.00 37.33	. В
	ATOM	1444	c	GLY	198	23.715	24.583	61.240	1.00 38.13	В
	ATOM	1445	ō	GLY	198	24.580	25.198	60.615	1.00 39.69	В
	MOTA	1446	N	LEU	199	23.530	23.275	61.098	1.00 37.34	В
70	MOTA	1447	CA	LEU	199	24.376	22.512	60.190	1.00 36.62	В
70	ATOM	1448	CB	LEU	199	24.218	21.006	60.444	1.00 34.70	В
	MOTA	1449	CG	LEU	199	25.067	20.058	59.588	1.00 33.44	В
	MOTA	1450		LEU	199	26.553	20.355	59.755	1.00 31.11	В
	MOTA	1451	CD2	LEU	199	24.767	18.634	59.994	1.00 32.49	В

	ATOM	1452	С	LEU	199		24.066	22.838	58.729	1.00 36.33	В
	MOTA	1453	0	LEU	199		22.971	22.550	58.228	1.00 35.86	В
	ATOM	1454	N	GLU	200		25.040	23.441	58.053	1.00 35.51	В
_	MOTA	1455	CA	GLU	200		24.896	23.815	56.653	1.00 37.46	В
5	MOTA	1456	CB	GLU	200		26.037	24.746	56.234	1.00 40.69	В
	ATOM	1457	CG	GLU	200		26.005	26.135	56.868	1.00 49.20	В
	MOTA	1458	CD	GLU	200	٠	24.757	26.925	56.502	1.00 51.96	В
	MOTA	1459		GLU	200		23.659	26.576	56.990	1.00 54.11	В
10	MOTA	1460	OE2	GLU	200		24.873	27.896	55.722	1.00 54.04	В
10	ATOM	1461	С	GLU	200		24.874	22.612	55.717	1.00 36.14	В
	MOTA	1462	.0	GLU	200		25.434	21.564	56.015	1.00 35.01	В
	MOTA	1463	N	GLU	201		24.217	22.787	54.575	1.00 35.47	В
	MOTA	1464	CA	GLU	201		24.124	21.752	53.559	1.00 34.36	В
16	MOTA	1465	CB	GLU	201		22.709	21.189	53.483	1.00 34.40	В
15	MOTA	1466	CG	GLU	201		22.207	20.582	54.773	1.00 34.93	В
	MOTA	1467	CD	GLU	201		20.816	19.998	54.626	1.00 36.86	В
	ATOM	1468		GLU	201		20.137	19.825	55.665	1.00 37.44	В
	MOTA	1469		GLU	201		20.408	19.710	53.476	1.00 36.10	В
20	MOTA	1470	C	GLU	201		24.479	22.393	52.226	1.00 34.09	В
20	MOTA MOTA	1471 1472	0	GLU	201 202		23.681 25.687	23.115	51.657 51.740	1.00 33.70	В
	MOTA	1473	N CA	ILE	202		26.130	22.127 22.689	50.472	1.00 33.17 1.00 32.42	В
	MOTA	1474	CB	ILE	202		27.679	22.715	50.472	1.00 32.42	В. В
	MOTA	1475		ILE	202		28.087	23.275	49.002	1.00 33.25	·B
25	ATOM	1476		ILE	202		28.286	23.582	51.465	1.00 33.81	В
	ATOM	1477		ILE	202		28.222	22.967	52.849	1.00 36.54	В
	MOTA	1478	c	ILE	202		25.572	21.888	49.305	1.00 31.15	В
	MOTA	1479	ō	ILE	202		25:703	20.678	49.257	1.00 33.14	В
	MOTA	1480	N	THR	203	•	24.948	22.583	48.361	1.00 29.99	. B
30	ATOM	1481	CA	THR	203		24.371	21.944	47.185	1.00 27.86	В
	MOTA	1482	CB	THR	203		23.228	22.804	46.572	1.00 27.52	В
	MOTA	1483		THR	203		22.157	22.925	47.516	1.00 27.78	В
	MOTA	1484	CG2	THR	203		22.701	22.174	45.284	1.00 26.79	В
	MOTA	1485	C	THR	203		25.448	21.741	46.130	1.00 27.11	В
35 ·	· MOTA	.1486	0	THR	203		26.217	22.637	45.853	1.00 26.94	В
	MOTA	1487	N	VAL	204		25.500	20.541	45.560	1.00 27.55	В
	MOTA	1488	CA'	VAL	204		26.467	20.222	44.517	1.00 27.42	В
	MOTA	1489	CB	VAL	204			. 18.859	44.781	1.00 25.01	В
40	MOTA	1490		VAL	204		28.393	18.718	43.941	1.00 23.11	В
40	ATOM	1491		VAL	204		27.468	18.729	46.250	1.00 23.76	В
	MOTA	1492	c	VAL	204		25.677	20.178	43.207	1.00 29.81	В
	ATOM	1493	0	VAL	204		24.887	19.261	42.983	1.00 30.56	В
	ATOM	1494	N	HIS	205		25.891	21.188	42.364	1.00 30.97	В
45	MOTA	1495	CA	HIS	205		25.197	21.318	41.079	1.00 33.24	В
-1 5	MOTA	1496	CB	HIS	205		25.199	22.792	40.649	1.00 33.42	В
	ATOM	1497 1498	CG	HIS	205		24.641	23.716	41.687	1.00 34.00	В
	MOTA MOTA	1499		HIS	205 205	٠	25.233 23.297	24.333 24.019	42.739 41.771	1.00 33.05	В
	MOTA	1500		HIS	205		23.297	24.777	42.832	1.00 33.23 1.00 33.03	B B
50	MOTA	1501		HIS	205		24.244	24.981	43.437	1.00 32.48	В
	ATOM	1502	c	HIS	205		25.790	20.450	39.969	1.00 33.72	В
	ATOM	1503	ŏ	HIS	205		25.084	20.022	39.061	1.00 32.22	В
	ATOM	1504	N	ASN	206	• •	27.094	20.201	40.048	1.00 35.23	. B
	ATOM	1505	CA	ASN	206		27.779	19.381	39.055	1.00 36.89	B
55 .	ATOM	1506	CB	ASN	206		28.178	20.229	37.837	1.00 37.95	В
	MOTA	1507	CG	ASN	206		28.999	21.455	38.213	1.00 41.34	В
	MOTA	1508	OD1	ASN	206		30.130	21.339	38.697	1.00 43.10	В
	ATOM	1509	ND2	ASN	206		28.428	22.641	37.993	1.00 38.53	В.
	MOTA	1510	C	ASN	206		29.007	18.712	39.666	1.00 36.43	В
60	MOTA	1511	0	ASN	206		29.233	18.805	40.864	1.00 36.95	В
	MOTA	1512	N	LYS	207		29.787	18.029	38.834	1.00 36.70	В
	MOTA	1513	CA	LYS	207		30.983	17.338	39.297	1.00 37.65	В
	MOTA	1514	CB	LYS	207		31.357	16.232	38.314	1.00 38.65	В
<i>C</i>	ATOM	1515	CG	LYS	207		31.892	16.726	36.977	1.00 41.42	В
65	ATOM	1516	CD	LYS	207		31.938	15.585	35.966	1.00 45.62	8
	ATOM	1517	CE	LYS	207		32.889	15.877	34.814	1.00 47.44	В
	ATOM	1518	NZ	LYS	207		34.314	15.937	35.262	1.00 47.37	В
	MOTA	1519	C	LYS	207		32.155	18.298	39.464	1.00 38.02	В
70	MOTA	1520	0	LYS	207		32.990	18.121	40.340	1.00 38.46	В
70	ATOM	1521	N	ASP	208		32.199	19.320	38.618	1.00 38.91	. В
	ATOM	1522	CA	ASP	208		33.264	20.313	38.667	1.00 40.47	В
	MOTA MOTA	1523 1524	CB CG	ASP ASP	208		33.316	21.061	37.338	1.00 42.51	В
	VI ON	1764	CO	nor	208	*	33.664	20.156	36.192	1.00 44.26	В

	MOTA	1525	ODI	ASP	208	33.297	20.470	35.041	1.00 44.33	В
	ATOM	1526		ASP	208	34.321	19.127	36.451	1.00 46.27	В
	MOTA	1527	Ċ	ASP	208	33.058	21.300	39.805	1.00 39.34	В
-	MOTA	1528	0	ASP	208	33.568	22.405	39.780	1.00 40.79	В
5	MOTA	1529	N	GLU	209	32.308	20.893	40.813	1.00 38.81	В
	MOTA	1530	CA	GLU	209	32.050	21.772	41.930	1.00 38.33	₿
	ATOM	1531	CB	GLU	209	30.604	22.260	41.866	1.00 39.47	В
	MOTA	1532	CG	GLU	209	30.278	23.400	42.805	1.00 42.87	В
10	ATOM	1533	CD	GLU	209	28.824		42.700	1.00 44.43	В
10	MOTA MOTA	1534 1535		GLU	209 209	28.373 28.135	24.134	41.573	1.00 42.49	В
	MOTA	1536	C	GLU	209	32.303	23.885 21.055	43.749 43.247	1.00 44.53	· B
	MOTA	1537	ŏ	GLU	209	32.147	21.649	44.316	1.00 37.83	В
	ATOM	1538	N	VAL	210	32.720	19.790	43.171	1.00 35.54	В
15	ATOM	1539	CA	VAL	210	32.954	19.011	44.384	1.00 32.37	В
	ATOM	1540	CB	VAL	210	32.679	17.485	44.158	1.00 31.94	В
	MOTA	1541		VAL	210	31.641	17.286	43.057	1.00 31.12	. В
•	MOTA	1542		VAL	210	33.961	16.749	43.842	1.00 30.76	В
20	MOTA	1543	c	VAL	210	34.342	19.173	44.991	1.00 29.97	В
20	MOTA	1544	0	VAL	210	34.482	19.206	46.207	1.00 29.98	В
	MOTA	1545	N	TYR	211	35.367	19.285	44.154	1.00 27.29	В
	MOTA ATOM	1546 1547	CB	TYR TYR	211 211	36.718 37.747	19.408 19.437	44.685	1.00 25.19	В
	MOTA	1548	CG	TYR	211	39.177	19.352	43.549 44.040	1.00 24.73 1.00 26.20	B B
25	MOTA	1549		TYR	211	39.601	18.278	44.824	1.00 27.98	B
	ATOM	1550		TYR	211	40.903	18.214	45.325	1.00 27.65	. B
	MOTA	1551		TYR	211 .	40.093	20.360	43.761	1.00 26.06	В
	MOTA	1552	CE2	TYR	211	41.398	20.308	44.257	1.00 26.72	В
20	MOTA	1553	CZ	TYR	211	41.797	19.233	45.041	1.00 29.28	В
30	MOTA	1554	OH	TYR	211	43.081	19.193	45.556	1.00 27.76	В
	MOTA	1555	C	TYR	211	36.864	20.635	45.573	1.00 24.67	₿
	MOTA MOTA	1556 1557	0	TYR	211	37.515	20.578	46.615	1.00 24.02	В
	ATOM	1558	N CA	GLN GLN	212 212	36.251 36.294	21.742 22.982	45.160 45.926	1.00 25.05	В
35	ATOM	1559	CB	GLN	212	35.508	24.082	45.224	1.00 24.24	B B
-	MOTA	1560	CG	GLN	212	36.375	25.051	44.459	1.00 36.14	В
	ATOM	1561	CD	GLN	212	35.625	26.311	44.048	1.00 40.99	В
	ATOM	1562		GLN	212	34.641	26.248	43.312	1.00 42.51	В
40	MOTA	1563	NE2	GLN	212	36.090	27.465	44.532	1.00 41.52	В
40	MOTA	1564	С	GLN	212	35.713	22.777	47.305	1.00 22.91	B
	MOTA	1565	0	GLN	212	36.285	23.206	48.299	1.00 23.35	В
	MOTA	1566	N	ILE	213	34.560	22.122	47.362	1.00 22.44	В
	MOTA MOTA	1567 1568	CA CB	ILE	213 213	33.905	21.876	48.640	1.00 22.31	В
45	ATOM	1569		ILE	213	32.595 31.910	21.095 20.947	48.472 49.828	1.00 20.76	В
••	ATOM	1570		ILE	213	31.675	21.821	47.492	1.00 21.01 1.00 20.79	B B
	ATOM	1571	CD1		213	30.457	21.012	47.071	1.00 22.47	В
	MOTA	1572	C	ILE	213	34.816	21.095	49.573	1.00 22.67	В
	MOTA	1573	0	ILE	213	34.863	21.366	50.764	1.00 23.38	В
50	MOTA	1574	N	LEU	214	35.539	20.126	49.020	1.00 24.93	В
	MOTA	1575	CA	LEU	214	36.455	19.307	49.811	1.00 26.22	В
	MOTA	1576	CB	LEU	214	36.965	18.129	48.972	1.00 27.09	В
	MOTA	·1577	CG	LEU	214	36.092	16.868	48.882	1.00 29.34	В
55	ATOM ATOM	1578 1579		LEU	214 214	34.618	17.235	48.836	1.00 30.24	В
55	MOTA	1580	CD2	LEU		36.491 37.621	16.059 20.149	47.649 50.314	1.00 30.55	B B
	ATOM		ò	LEU	214		19.994	51.444	1.00 26.33	B
	MOTA	1582	N	GLU	215	38.108	21.049	49.464	1.00 25.83	В
	MOTA	1583	CA	GLU	215	39.215	21.930	49.834	1.00 24.69	B
60	MOTA	1584	CB	GLU	215	39.586	22.830	48.655	1.00 23.60	В
	MOTA	1585	CG	GLU	215	40.814	22.380	47.882	1.00 22.50	В
	MOTA	1586	CD	GLU	215	40.907	23.030	46.511	1.00 23.11	В
	MOTA	1587		GLU	215	42.047	23.251	46.040	1.00 20.98	B
65	ATOM	1588		GLU	215	39.839	23.306	45.913	1.00 20.38	. В
O)	MOTA	1589	C	GLU	215	38.837	22.784	51.040	1.00 23.82	В
	MOTA MOTA	1590 1591	O N	GLU - LYS	215 216	39.636	22.960	51.967 51.033	1.00 23.91	B
	ATOM	1592	CA	LYS	216	37.617 37.152	23.306 24.135	52.129	1.00 22.14	В
	MOTA	1593	CB	LYS	216		24.135	52.129	1.00 24.81	B B
70	ATOM	1594	CG	LYS	216	35.875	25.760	50.637	1.00 25.88	B
	MOTA	1595	CD	LYS	216	34.492	26.263	50.229	1.00 40.73	В
	MOTA	1596	CE	LYS	216	34.591	27.386	49.208	1.00 42.22	В
	MOTA	1597	NZ	LYS	216	35.405	27.007	48.007	1.00 44.86	В

											,
•	MOTA	1598	C	LYS	216		37.066	23.327	53.417	1.00 24.49	В
	MOTA	1599	0	LYS	216		37.497	23.790	54.475	1.00 25.43	В
	MOTA	1600	N	GLY	217		36.525	22.117	53.325	1.00 22.80	В
5	MOTA	1601	CA	GLY	217		36.427	21.282	54.498	1.00 21.61	В
,	MOTA	1602	C	GLY	217		37.813	21.056	55.063	1.00 21.73	В
	MOTA .	1603	0	GLY	217		38.019	21.154	56.273	1.00 21.45	В
	MOTA	1604	N	ALA	218 218		38.770	20.770	54.182	1.00 19.63	В
•	MOTA	1606	CA	ALA ALA	218		40.146	20.522	54.607	1.00 20.23	В
10	ATOM	1607	CB C	ALA	218		40.720	20.194 21.717	53.402 55.358	1.00 20.86	В
10	MOTA	1608	.0	ALA	218		41.151	21.588	56.500	1.00 19.43	В
	ATOM	1609	N	ALA	219		40.725	22.877	54.706	1.00 21.17 1.00 19.70	B B
	ATOM	1610	CA	ALA	219		41.248	24.111	55.299	1.00 19.70	В
•	ATOM	1611	CB	ALA	219		40.928	25.296	54.400	1.00 17.46	В
15	MOTA	1612	Ċ	ALA	219		40.672	24.357	56.675	1.00 18.82	В
_	MOTA	1613	ō	ALA	219		41.394	24.630	57.621	1.00 19.06	В
•	ATOM	1614	N	LYS	220		39.355	24.266	56.778	1.00 19.83	В
	MOTA	1615	CA	LYS	220		38.698	24.501	58.049	1.00 21.65	В
	MOTA	1616	CB	LYS	220		37.179	24.475	57.867	1.00 22.34	В
20	MOTA	1617	CG	LYS	220		36.416	24.906	59.101	1.00 25.89	В
	MOTA	1618	CD	LYS	220		35.002	25.363	58.759	1.00 28.36	В
	ATOM	1619	CE	LYS	220		34.296	25.886	60.002	1.00 28.81	В
	atom	1620	NZ	LYS	220		32.888	26.286	59.732	1.00 27.62	В
25	ATOM	1621	Ç	LYS	220		39.145	23.486	59.101	1.00 21.92	В
25	MOTA	1622	0	LYS	220		39.199	23.807	60.278	1.00 23.01	В
	MOTA	1623	N	ARG	221		39.478	22.268	58.672	1.00 21.66	В
	ATOM	1624	CA	ARG	221		39.934	21.223	59.596	1.00 20.06	В
	MOTA	1625	CB	ARG	221		40:015	19.878	58.882	1.00 22.12	В
30	MOTA MOTA	1626 1627	CG	ARG ARG	221		38.739	19.076	58.916	1.00 23.91	В
50	ATOM	1628	CD NE	ARG	221 221		38.952 37.777	17.787 16.929	58.173	1.00 26.21	В
	ATOM	1629	CZ	ARG	221		37.620	15.882	58.203 57.407	1.00 27.96 1.00 27.08	B B
•	ATOM	1630	NH1		221		38.571	15.583	56.529	1.00 27.08	В
	ATOM	1631	NH2		221		36.519	15.145	57.491	1.00 27.49	В
35	ATOM	.1632	c	ARG	221		41.301	21.562	60.167	1.00 18.78	В
	ATOM	1633	ō	ARG	221		41.623	21.206	61.315	1.00 16.42	В
	MOTA	1634	N	THR	222		42.101	22.238	59.350	1.00 15.19	В
	ATOM	1635	CA	THR	222		43.433	22.659	59.741	1.00 15.22	В
	MOTA	1636	CB	THR	222		44.119	23.409	58.593	1.00 16.99	В
40	ATOM	1637	OG1	THR	222		44.121	22.573	57.424	1.00 16.46	В
	ATOM	1638		THR	222		45.534	23.796	58.977	1.00 14.73	В
	MOTA	1639	Ç	THR	222		43.323	23.601	60.928	1.00 16.64	В
	MOTA	1640	0	THR	222		44.046	23.461	61.920	1.00 16.06	В
45	ATOM	1641	N	THR	223		42.405	24.559	60.828	1.00 16.39	В
47	MOTA	1642	CA	THR	223		42.202	25.515	61.902	1.00 17.40	В
	ATOM ATOM	1643 1644	CB	THR THR	223 223		41.160	26.603	61.519	1.00 18.18	В
	MOTA	1645		THR	223		39.839 41.268	26.125	61.780	1.00 22.16	В
	ATOM	1646	C ·	THR	223		41.708	26.953 24.757	60.048 63.134	1.00 1B.76 1.00 17.96	B B
50	ATOM	1647	ŏ	THR	223		42.078	25.083	64.253	1.00 17.30	В
	ATOM	1648	N	ALA	224		40.875	23.743	62.916	1.00 17.09	В
	ATOM	1649	CA	ALA	224		40.348	22.953	64.027	1.00 17.61	В
	MOTA	1650	CB	ALA	224	٠.	39.349	21.902	63.520	1.00 17.42	B
	MOTA	1651	C	ALA	224		41.503	22.268	64.744	1.00 16.75	В
55	ATOM	1652	0	ALA	224		41.588	22.284	65.979	1.00 13.71	В
	MOTA	1653	N	ALA	225		42.384	21.663	63.950	1.00 16.23	В
	MOTA	1654	CA	ALA	225		43.551	20.980	64.486	1.00 15.92	В
	MOTA	1655	CB	ALA	225		44.391	20.426	63.346	1.00 14.25	В
4۸	MOTA	1656	C	ALA	225		44.376	21.956	65.332	1.00 16.42	В
60	MOTA	1657	0	ALA	225		44.983	21.566	66.329	1.00 14.18	В
	MOTA	1658	N	THR	226		44.385	23.231	64.931	1.00 18.14	В
	MOTA	1659	CA	THR	226		45.135	24.261	65.666	1.00 18.36	В
	MOTA	1660	CB	THR	226		45.205	25.606	64.894	1.00 19.59	В
65	MOTA MOTA	1661 1662		THR THR	226		45.994	25.445	63.705	1.00 20.89	В
55	ATOM	1663	C	THR	226 226		45.821 44.507	26.696 24.541	65.775	1.00 18.63	В
	ATOM	1664	0	THR	226		45.214	24.765	67.024 68.000	1.00 19.56 1.00 22.00	В
	ATOM	1665	N	LEU	227		43.178	24.765	67.074	1.00 22.00	B B
_	ATOM	1666	CA	LEU	227		42.427	24.798	68.297	1.00 19.70	В
70	ATOM	1667	СВ	LEU	227		41.011	25.291	67.943	1.00 22.99	В
	ATOM	1668	CG	LEU	227		40.728	26.794	67.875	1.00 28.11	В
	MOTA	1669		LEU	227		41.162	27.422	69.202	1.00 28.40	В
	MOTA	1670	CD2	LEU	227		41.452	27.445	66.677	1.00 27.33	В

	ATOM	1671	С	LEU	227	42.279	23.627	69.269	1.00 19.64	В
	ATOM	1672	0	LEU	227	42.384	23.801	70.480	1.00 17.11	B
	ATOM	1673	N	MET	228	42.021	22.440	68.727	1.00 21.48	В
	ATOM	1674	CA	MET	228	41.807	21.253	69.557	1.00 21.62	В
5										
J	MOTA	1675	CB	MET	228	40.465	20.627	69.174	1.00 21.31	В
	ATOM	1676	CG	MET	228	39.286	21.542	69.510	1.00 22.62	В
	ATOM	1677	SD	MET	228	37.764	21.286	68.570	1.00 28.36	В
	ATOM	1678	CE	MET	228	37.979	22.463	67.223	1.00 25.23	В
	ATOM	1679	C	MET	228	42.936		69.472	1.00 19.55	
10										В
10	ATOM	1680	0	MET	228	43.364	19.884	68.392	1.00 19.08	В
	MOTA	1681	N	ASN	229	43.404	19.764	70.628	1.00 19.30	В
	MOTA	1682	CA	ASN	229	44.496	18.790	70.683	1.00 21.72	B
	ATOM	1683	CB	ASN	229	44.902	18.512	72.140	1.00 21.27	В
	MOTA	1684	CG	ASN	229	45.124	19.786	72.952	1.00 23.92	В
15										
13	ATOM	1685	OD1	ASN	229	45.493	20.829	72.413	1.00 26.36	В
	ATOM	1686	ND2	ASN	229	44.913	19.694	74.262	1.00 18.44	В
	ATOM	1687		ASN	229			69.993	1.00 21.18	
			C			44.165	17.460			В
•	ATOM	1688	0	ASN	229	43.071	16.927	70.153	1.00 21.11	В
	MOTA	1689	N	ALA	230	45.129	16.945	69.231	1.00 20.55	В
20										
20	ATOM	1690	CA	ALA	230	44.975	15.683	68.510	1.00 21.88	В
	MOTA	1691	CB	ALA	230	45.172	14.502	69.466	1.00 22.05	В
	MOTA	1692	C	ALA	230	43.599	15.601	67.869	1.00 21.44	В
	MOTA	1693	0	ALA	230	42.925	14.588	67.974	1.00 23.20	В
	ATOM	1694	N	TYR	231	43.197	16.667	67.191	1.00 20.11	В
25	ATOM									
25		1695	CA	TYR	231	41.878	16.708	66.568	1.00 21.54	• В
	ATOM	1696	CB	TYR	231	41.637	18.103	65.968	1.00 19.36	. В
	ATOM	1697	CG	TYR	231	40.280	18.276	65.322	1.00 14.20	В
	MOTA	1698		TYR	231	40.106	18.061	63.956	1.00 10.71	В
	MOTA	1699	CE1	TYR	231	38.852	18.173	63.369	1.00 9.05	В
30	ATOM	1700	CD2	TYR	231	39.159	18.613	66.085	1.00 14.00	В
50										
	MOTA	1701	CE2	TYR	231	37.900	18.725	65.503	1.00 11.47	В
	MOTA	1702	CZ	TYR	231	37.757	18.505	64.152	1.00 9.28	В
	ATOM	1703	ОН	TYR	231.	36.522	18.626	63.583	1.00 11.26	В
~~	ATOM	1704	С	TYR	231	41.603	15.614	65.526	1.00 22.31	В
35	MOTA	1705	0	TYR	231	40.611	14.889	65.630	1.00 23.44	В.
	ATOM	1706	N	SER	232	42.481	15.482	64.538	1.00 21.31	
										В
	MOTA	1707	CA	SER	232	42.286	14.487	63.486	1.00 21.21	В
	MOTA	1708	CB	SER	232	43.382	14.614	62.424	1.00 19.70	В
	MOTA	1709	ŌG	SER	232	44.658	14.355			
40								62.980	1.00 22.28	B
40	MOTA	1710	С	SER	232	42.245	13.046	63.983	1.00 20.84	В
	ATOM	1711	0	SER	232	41.718	12.165	63.303	1.00 21.67	В
	MOTA	1712	N	SER	233	42.788	12.805	65.166	1.00 18.82	В
	ATOM	1713	CA	SER	233	42.801	11.447	65.670	1.00 16.78	В
	ATOM	1714	CB	SER	233	44.189	11.108	66.222	1.00 14.92	В
45										
73	MOTA	1715	OG	SER	233	44.295	11.465	67.587	1.00 15.42	В
	MOTA	1716	С	SER	233	41.745	11.193	66.741	1.00 17.60	В
	MOTA	1717	0	SER	233	41.365	10.067	66.964	1.00 18.14	В
	MOTA	1718	N	ARG	234	41.267	12.253	67.392	1.00 18.41	В
	MOTA	1719	CA	ARG	234	40.266	12.113	68.450	1.00 18.22	В
50	ATOM	1720	CB	ARG	234	40.716	12.874	69.703	1.00 20.85	
50										В
	MOTA	1721	CG	ARG	234	41.207	11.975	70.809	1.00 26.63	В
	MOTA	1722	CD	ARG	234	42.603	12.340	71.282	1.00 28.86	В
	ATOM	1723	NE	ARG	234	42.624	13.522	72.138	1.00 28.89	В
	ATOM	1724	CZ	ARG	234	43.641	13.853	72.927	1.00 30.32	В
55	ATOM	1725	NH1	ARG	234	44.724	13.089	72.969	1.00 29.87	В
-	ATOM	1726	NH2		234					
						43.571	14.941	73.683	1.00 29.28	В
	ATOM	1727	С	ARG	234	38.858	12.559	68.065	1.00 18.79	В
	MOTA	1728 -	0	ARG	234	37.986	12.639	68.914	1.00 18.55	В
<i>(</i> 0	MOTA	1729	N	SER	235	38.641	12.826	66.780	1.00 19.09	В
60	MOTA	1730	CA	SER	235	37.339	13.278	66.307	1.00 18.40	В
	MOTA	1731	CB	SER	235	37.477	14.654	65.655	1.00 16.08	B
	MOTA	1732	OG	SER	235	38.275	14.584	64.481	1.00 13.92	В
	MOTA	1733	С	SER	235	36.694	12.314	65.312	1.00 18.89	В
	ATOM	1734	ŏ	SER	235					
65						37.379	11.637	64.558	1.00 18.57	В
65	MOTA	1735	N	HIS	236	35.363	12.284	65.323	1.00 20.05	В
	MOTA	1736	CA	HIS	236	34.571	11.445	64.427	1.00 20.67	В
	MOTA	1737	CB	HIS	236	33.409	10.800	65.186	1.00 21.89	В
	ATOM .	1738	CG	HIS	236	33.819	10.092	66.439	1.00 22.09	В
	ATOM	1739	CD2		236	33.733	10.462	67.740	1.00 22.95	В
70										
10	MOTA	1740	ND1		236	34.406	8.847	66.433	1.00 22.44	В
	MOTA	1741	CE1	HIS	236	34.663	8.480	67.677	1.00 24.61	В
	MOTA	1742	NE2		236	34.265	9.441	68.489		
									1.00 23.56	В
	ATOM	1743	С	HIS	236	33.994	12.353	63.345	1.00 21.61	В

	ATOM	1744	0	HIS	236	33.373	13.368	63.658	1.00 22.50	В
	MOTA	1745	N	SER	237	34.195	12.000	62.080	1.00 20.87	В
	MOTA	1746	CA	SER	237	33.673	12.813	60.992	1.00 21.41	В
~	MOTA	1747	CB	SER	237	34.811	13.241	60.061	1.00 21.79	В
5	MOTA	1748	OG	SER	237	35.388	12.121	59.411	1.00 21.23	В
	MOTA	1749	С	SER	237	32.618	12.049	60.201	1.00 22.61	В
	MOTA	1750	ō	SER	237	32.863	10.939	59.749	1.00 23.35	В
	ATOM	1751	N	VAL	238	31.440	12.648	60.053	1.00 21.59	
										В
1Λ	MOTA	1752	CA	VAL	238	30.348	12.022	59.313	1.00 20.89	В
10	MOTA	1753	CB	VAL	238	29.106	11.821	60.234	1.00 22.16	В
	MOTA	1754	· CG1	VAL	238	28.807	13.104	60.977	1.00 24.21	В
	MOTA	1755	CG2	VAL	238	27.886	11.395	59.419	1.00 18.41	В
	ATOM	1756	C	VAL	238	29.967	12.872	58.103	1.00 18.95	В
•	ATOM	1757		VAL	238	29.157	13.772	58.205	1.00 18.39	В
15										
13	MOTA	1758	N	PHE	239	30.586	12.577	56.962	1.00 19.38	В
	MOTA	1759	CA	PHE	239	30.329	13.295	55.712	1.00 19.10	В
	MOTA	1760	CB	PHE	239	31.501	13.115	54.735	1.00 16.63	В
	MOTA	1761	CG	PHE	239	31.413	13.986	53.501	1.00 13.65	В
	MOTA	1762	CD1	PHE	239	30.443	13.752	52.521	1.00 13.62	В
20	ATOM	1763		PHE	239	32.307	15.029	53.316	1.00 11.10	В
	ATOM	1764		PHE	239					
						30.375	14.557	51.367	1.00 11.04	В
	ATOM	1765		PHE	239	32.248	15.836	52.174	1.00 11.49	В,
	MOTA	1766	CZ	PHE	239	31.281	15.598	51.196	1.00 10.13	В
~-	MOTA	1767	С	PHE	239	29.072	12.709	55.089	1.00 20.70	· B
25	ATOM	1768	0	PHE	239	29.088	11.581	54.635	1.00 21.65	В
	ATOM	1769	N	SER	240	27.992	13.487	55.056	1.00 19.79	В
	ATOM	1770	CA	SER	240	26.737	12.999	54.489	1.00 20.02	В
	ATOM	1771	CB	SER	240	25.568	13.303	55.430	1.00 17.99	В
20	MOTA	1772	OG	SER	240	25.714	12.651	56.682	1.00 13.88	· В
30	MOTA	1773	С	SER	240	26.424	13.552	53.104	1.00 21.86	В
	MOTA	1774	0	SER	240	26.721	14.684	52.796	1.00 22.91	В
	MOTA	1775	N	VAL	241	25.818	12.720	52.271	1.00 23.30	В
	MOTA	1776	CA	VAL	241	25.448	13.130	50.932	1.00 24.80	В
	ATOM	1777	CB	VAL	241	26.432	12.581	49.884		
35 ⁻									1.00 24.40	В
JJ	MOTA	1778		VAL	241	26.805	11.139	50.226	1.00 26.22	В
	ATOM	1779	CG2		241	25.807	12.668	48.494	1.00 19.02	В
	MOTA	1780	C	VAL	241	24.035	12.646	50.619	1.00 26.53	В
	MOTA	1781	0	VAL	241	23.806	11.465	50.433	1.00 27.95	В
	MOTA	1782	N	THR	242	23.093	13.582	50.586	1.00 28.63	В
40	MOTA	1783	CA	THR	242	21.698	13.287	50.311	1.00 30.95	B
	ATOM	1784		THR	242					
			CB			20.779	14.186	51.164	1.00 32.05	В
	ATOM	1785	0G1	THR	242	20.997	13.901	52.555	1.00 33.54	В
•	ATOM	1786	CG2	THR	242	19.319	13.939	50.825	1.00 34.70	В
	MOTA	1787	С	THR	242	21.393	13.490	48.828	1.00 32.32	В
45	ATOM	1788	0	THR	242	21.845	14.451	48.213	1.00 33.97	В
	ATOM	1789	N	ILE	243	20.628	12.573	48.250	1.00 33.03	В
	ATOM	1790	CA	ILE	243	20.293	12.660	46.837	1.00 33.83	В
	ATOM	1791	CB	ILE	243	20.912	11.493	46.052	1.00 33.37	В
50	MOTA	1792		ILE	243	20.732	11.719	44.561	1.00 32.82	В
50	MOTA	1793		ILE	243	22.395	11.361	46.400	1.00 34.30	В
	ATOM	1794	CD1	ILE	243	23.071	10.176	45.750	1.00 35.23	В
	MOTA	1795	С	ILE	243	18.789	12.635	46.604	1.00 35.12	В
	ATOM	1796	0	ILE	243	18.175	11.581	46.655	1.00 34.29	В
	ATOM	1797	N	HIS	244	18.197	13.803	46.364	1.00 37.02	В
55	ATOM	1798		HIS		16.766				
55			CA		244		13.878	46.097	1.00 38.10	В
	MOTA	1799	CB	HIS	244	16.214	15.280	46.390	1.00 40.10	В
	MOTA	1800	CG	HIS	244	16.190	15.635	47.845	1.00 42.80	В
	ATOM	1801	CD2	HIS	244	15.219	15.493	48.781	1.00 43.38	В.
	ATOM	1802	ND1	HIS	244	17.271	16.192	48.496	1.00 44.55	В
60 ·	MOTA	1803		HIS	244	16.968	16.376	49.770	1.00 44.18	В
	ATOM	1804		HIS	244	15.729				
							15.960	49.968	1.00 43.01	В
	ATOM	1805	C	HIS	244	16.569	13.545	44.624	1.00 38.58	В
	MOTA	1806	0	HIS	244	17.113	14.216	.43 .754	1.00 38.74	В
	ATOM	1807	N	MET	245	15.790	12.500	44.357	1.00 38.78	В
65	MOTA	1808	CA	MET	245	15.534	12.056	42.991	1.00 38.49	В
	MOTA	1809	CB	MET	245	16.081	10.646	42.791	1.00 35.74	В
	ATOM	1810	CG	MET	245	17.579	10.552	42.978	1.00 34.03	В
	MOTA	1811	SD	MET	245	18.110			1.00 34.03	
							8.870	43.218		В
70	MOTA	1812	CE	MET	245	17.855	8.694	44.996	1.00 26.04	В
/U	MOTA	1813	C	MET	245	14.058	12.083	42.618	1.00 39.24	В
	MOTA	1814	0	MET	245	13.193	11.814	43.439	1.00 39.24	В
	ATOM	1815	N	LYS	246	13.791	12.409	41.358	1.00 39.88	В
	ATOM	1816	CA	LYS	246	12.430	12.477	40.855	1.00 40.90	В
					-		**			_

	MOTA	1817	CB	LYS	246	11.910	13.916	40.915	1.00 42.86	В
	MOTA	1818	CG	LYS	246	10.453	14.080	40.467	1.00 45.41	В
	MOTA	1819	CD	LYS	246	10.140	15.516	40.018	1.00 47.23	В
	ATOM	1820	CE	LYS	246	10.383	16.538	41.134	1.00 49.08	В
5	ATOM	1821	NZ	LYS	246	10.267	17.954	40.659	1.00 47.64	
,										В
	MOTA	1822	C.	LY\$	246	12.406	11.994	39.414	1.00 41.15	В
	MOTA	1823	0	LYS	246	13.084	12.547	38.552	1.00 40.37	В
	MOTA	1824	N	GLU	247	11.622	10.954	39.163	1.00 40.39	В
. 1	MOTA	1825	CA	GLU	247	11.496	10.414	37.821	1.00 40.56	В
10	MOTA	1826	CB	GLU	247	12.010	8.977	37.769	1.00 39.14	В
10										
	MOTA	1827	CG	GLU	247	11.479	8.090	38.866	1.00 37.23	В
	ATOM	1828	CD	GLU	247	12.390	6.916	39.118	1.00 36.86	В
	ATOM	1829		GLU	247			40.021		
						12.094	6.104		1.00 36.22	В
	MOTA	1830	OE2	GLU	247	13.410	6.813	38.406	1.00 36.77	В
15	MOTA	1831	С	GLU	247	10.039	10.469	37.402	1.00 40.31	В
	MOTA	1832	0	GLU	247	9.142	10.304	38.220	1.00 39.86	В
	MOTA	1833	N	THR	248	9.820	10.720	36.117	1.00 40.83	B
•	MOTA	1834	CA	THR	248	8.480	10.826	35.569	1.00 40.95	В
20	MOTA	1835	CB	THR	248	8.339	12.123	34.736	1.00 40.97	В
20	MOTA	1836	OG1	THR	248	8.804	13.238	35.507	1.00 41.15	В
	MOTA	1837	CG2	THR	248	6.886	12.363	34.358	1.00 40.88	В
	ATOM .	1838	С	THR	248	8.143	9.625	34.690	1.00 40.36	В
	ATOM	1839	0	THR	248	8.799	9.380	33.684	1.00 40.50	В
	MOTA	1840	N	THR	249	7.111	8.885	35.086	1.00 39.94	В
25										
43	MOTA	1841	CA	THR	249	6.661	7.712	34.341	1.00 39.13	• В
	ATOM	1842	CB	THR	249	5.537	6.976	35.086	1.00 39.64	. В
	ATOM	1843		THR	249	4.307	7.686	34.897	1.00 37.39	В
	ATOM	1844	CG2	THR	249	5.846	6.894	36.575	1.00 38.52	В
	ATOM	1845	С	THR	249	6.115	8.132	32.980	1.00 39.50	В
30	ATOM		ō							
50		1846		THR	249	5.943	9.311	32.713	1.00 39.71	В
	MOTA	1847	N	ILE	250	5.841	7.148	32.129	1.00 40.73	В
	ATOM	1848	CA	ILE	250	5.307	7.398	30.794	1.00 40.49	В
	MOTA	1849	CB	ILE	250 .	5.292	6.095	29.944	1.00 37.78	В
	ATOM	1850	CG2	ILE	250	4.244	5.135	30.472	1.00 37.42	В
35	ATOM	1851		ILE	250	4.999	6.421	28.479	1.00 35.79	В .
-										
	MOTA	1852	CDI	ILE	250	5.125	5.238	27.552	1.00 33.62	В
	MOTA	1853	С	ILE	250	3.892	7.963	30.905	1.00 42.55	В
	MOTA	1854	0	ILE	250	3.361	8.534	29.953		
									1.00 43.05	В
4.0	MOTA	1855	N	ASP	251	3.296	7.800	32.084	1.00 44.44	В
40	MOTA	1856	CA	ASP	251	1.947	8.286	32.357	1.00 46.93	B
. •										
	MOTA	1857	CB	ASP	251	1.215	7.318	33.290	1.00 47.07	В
	MOTA	1858	CG	ASP	251	0.494	6.221	32.539	1.00 47.33	В
	ATOM	1859	OD1	ASP	251	0.034	5.257	33.190	1.00 47.89	В
45	MOTA	1860	ODZ	ASP	251	0.381	6.325	31.298	1.00 45.62	В
45	ATOM	1861	С	ASP	251	1.965	9.675	32.987	1.00 48.37	В
	ATOM	1862	Ō	ASP	251	0.933	10.175	33.424		
									1.00 49.52	В
	MOTA	1863	N	GLY	252	3.145	10.286	33.038	1.00 49.00	В
	MOTA	1864	CA	GLY	252	3.275	11.612	33.609	1.00 48.84	В
	MOTA	1865		GLY	252					
50			Ç			3.432	11.634	35.117	1.00 49.43	В
20	MOTA	1866	0	GLY	252	3.856	12.638	35.675	1.00 49.95	В
	MOTA	1867	N	GLU	253	3.093	10.538	35.787	1.00 49.54	В
	ATOM	1868	CA	GLU	253	3.219	10.499	37.237	1.00 50.34	
										В
	MOTA	1869	CB	GLU	253	2.693	9.183	37.797	1.00 51.72	В
	MOTA	1870	CG	GLU	253	2.753	9.136	39.309	1.00 55.44	В
55	MOTA	1871	CD	GLU	253					
J J						2.605	7.734	39.856	1.00 57.73	В
	MOTA	1872	OE1	GLU	253	2.703	7.561	41.091	1.00 59.23	В
	MOTA	1873	OE2	GLII	253	2.400	6.805	39.048	1.00 59.21	В
	MOTA	1874	С	GLU	253	4.671	10.678	37.661	1.00 49.73	В
	ATOM	1875	0	GLU	253	5.582	10.326	36.930	1.00 49.04	В
60	MOTA	1876	N	GLU	254	4.878	11.229	38.851	1.00 49.71	
										В
	MOTA	1877	CA	GLU	254	6.230	11.445	39.346	1.00 50.40	В
	MOTA	1878	CB	GLU	254	6.452	12.927	39.629	1.00 51.91	В
	ATOM	1879	CG	GLU	254	7.036		38.448	1.00 56.74	
							13.680			В
	MOTA	1880	CD	GLU	254	6.579	15.124	38.397	1.00 59.63	B
65	ATOM	1881	OE1		254	6.444	15.739	39.479	1.00 61.46	В
	ATOM	1882	OE2		254	6.363	15.642	37.276	1.00 60.48	В
	MOTA	1883	С	GLU	254	6.562	10.614	40.578	1.00 48.68	В
	MOTA	1884	ō	GLU	254	5.812	10.579	41.546	1.00 47.25	
										В
70	MOTA	1885	N	LEU	255	7.703	9.938	40.517	1.00 47.02	В
70	MOTA	1886	CA	LEU	255	8.157	9.094	41.609	1.00 45.92	В
	ATOM	1887	CB	LEU	255	8.566				
							7.722	41.067	1.00 45.31	В
	MOTA	1888	CG	LEU	255	7.647	7.080	40.016	1.00 44.40	В
	MOTA	1889	CD1		255	8.308	5.837	39.454	1.00 43.92	В
	-				-	·				-

	MOTA	1890	CD2	LEU	255	6.294	6.747	40.621	1.00 43.09	В
	MOTA	1891		LEU	255	9.353				В
			Č				9.780	42.250	1.00 46.31	
	MOTA	1892	0	LEU	255	10.346	10.044	41.580	1.00 46.88	В
_	MOTA	1893	N	VAL	256	9.255	10.069	43.545	1.00 46.34	В
5	ATOM	1894	CA	VAL	256	10.343	10.739	44.254	1.00 46.32	В
_	ATOM	1895	CB	VAL	256	9.837	12.012	44.988	1.00 46.60	В
	ATOM		CG1		256	9.447	13.075	43.971	1.00 46.43	В
	MOTA	1897	CG2	VAL	256	8.642	11.679	45.870	1.00 46.46	В
	ATOM	1898	C	VAL	256	11.049	9.835	45.258	1.00 45.32	В
10	ATOM	1899	ō	VAL	256					
10			_			10.428	9.287	46.158	1.00 45.96	В
	MOTA	1900	. N	LYS	257	12:359	9.687	45.077	1.00 44:55	В
	MOTA	1901	CA	LYS	257	• 13.190	8.865	45.951	1.00 42.39	В
	MOTA	1902	CB	LYS	257	13.997	7.852	45.133	1.00 43.00	В
	MOTA	1903	CG	LYS	257	13.170	6.932	44.261	1.00 41.72	В
15										
IJ	MOTA	1904	CD	LYS	257	14.058	6.001	43.457	1.00 38.34	В
	MOTA	1905	CE	LYS	257	14.956	6.771	42.514	1.00 37.62	В
•	ATOM	1906	NZ	LYS	257	15.665	5.873	41.563	1.00 37.38	В
	ATOM	1907	С	LYS	257	14.161	9.755	46.705	1.00 40.94	В
	ATOM	1908			257					
20			0	LYS		14.545	10.802	46.220	1.00 42.05	В
20	MOTA	1909	N	ILE	258	14.557	9.322	47.893	1.00 38.70	В
	ATOM	1910	CA	ILE	258	15.498	10.082	48.699	1.00 35.70	В
	ATOM	1911	CB	ILE	258	14.790	10.816	49.850	1.00 36.93	В
	ATOM	1912		ILE	258	15.811	11.596	50.667	1.00 37.53	В.
25	ATOM	1913		ILE	258	13.729	11.767	49.291	1.00 38.43	.В
25	ATOM	1914	CD1	ILE	258	12.932	12.500	50.363	1.00 38.30	В
	ATOM	1915	С	ILE	258	16.541	9.142	49.285	1.00 33.73	В
	ATOM	1916	Ó	ILE	258	16.257	8.388	50.209	1.00 32.97	В
	ATOM	1917		GLY	259	17:746				
			N				9.186	48.731	1.00 31.67	- В
20	MOTA	1918	CA	GLY	259	18.815	8.338	49.219	1.00 30.51	. В
30	ATOM	1919	С	GLY	259	19.874	9.136	49.956	1.00 29.55	В
	ATOM	1920	0	GLY	259	20.363	10.138	49.442	1.00 30.38	В
	ATOM	1921	N	LYS	260	20.230	8.692	51.159	1.00 27.15	В
	ATOM	1922		LYS						
			CA		260	21.239	9.377	51.958	1.00 26.83	В
25	MOTA	1923	CB	LYS	260	20.603	9.940	53.240	1.00 24.21	В
35	MOTA	.1924	CG	LYS	260	21.518	10.858	54.037	1.00 19.17	В
	ATOM	1925	CD	LYS	260	20.833	11.362	55.289	1.00 17.68	В
	MOTA	1926	CE	LYS	260					
						21.768	12.219	56.124	1.00 16.42	В
	MOTA	1927	NZ	LYS	260	21.115	12.662	57.378	1.00 16.56	В
	MOTA	1928	С	LYS	260	22.394	8.437	52.318	1.00 27.97	В
40	ATOM	1929	0	LYS	260	22.184	7.357	52.864	1.00 30.85	В
-	ATOM	1930	N	LEU	261	23.616	8.859	52.011	1.00 26.40	В
	ATOM	1931	CA	LEU	261	24.792	8.056	52.306	1.00 24.54	В
	ATOM	1932	CB	LEU	261	25.587	7. 830	51.019	1.00 23.41	В
	ATOM	1933	CG	LEU	261	26.989	7.243	51.175	1.00 23.40	В
45	ATOM	1934	CD1	LEU	261	26.922	5.920	51.941	1.00 20.72	В
	MOTA	1935		LEU	261	27.599	7.045	49.798	1.00 20.51	В
	MOTA									
		1936	Ç,	LEU	261	25.685	8.715	53.362	1.00 23.98	В
	MOTA	1937	0	LEU	261	26.117	9.836	53.198	1.00 22.95	В
	MOTA	1938	N	ASN	262	25.953	8.000	54.448	1.00 22.99	В
50	MOTA	1939	CA	ASN	262	26.799	8.529	55.511	1.00 21.81	В
	MOTA	1940	CB	ASN	262	26.138	8.303	56.874	1.00 19.98	В
	MOTA	1941	CG	ASN	262	24.730				
							8.872	56.945	1.00 24.40	В
	MOTA	1942		ASN	262	23.770	8.135	57.124	1.00 24.74	В
	ATOM	1943	ND2	ASN	262	24.606	10.189	56.807	1.00 20.69	В
55	ATOM	1944	С	ASN	262	28.192	7.879	55.494	1.00 21.73	В
	ATOM	1945	0	ASN	262	28.314	6.680	55.589	1.00 20.91	В
	ATOM	1946					8.691			
				LEU	263	29.238		55.348		В
	ATOM	1947	CA	LEU	263	30.611	8.191	55.338	1.00 20.99	₿.
	ATOM	1948	CB	LEU	263	31.360	8.750	54.136	1.00 19.60	В
60 ·	ATOM	1949	CG	LEU	263	30.578	8.470	52.856	1.00 20.68	В
	ATOM	1950		LEU	263	31.187	9.220	51.710	1.00 22.18	
										В
	MOTA	1951		LEU	263	30.557	6.972	52.584	1.00 20.91	В
	ATOM	1952	С	LEU	263	31.262	8.650	56.630	1.00 21.08	В
	MOTA	1953	0	LEU	263	31.631	9.793	56.753	1.00 20.87	В
65	ATOM	1954	N	VAL	264	31.397	7.734	57.586	1.00 22.31	B
	ATOM	1955	CA	VAL	264	31.964	8.048	58.901	1.00 22.41	В
	MOTA	1956	СВ	VAL	264	31.119	7.378	60.042	1.00 22.70	В
	ATOM	1957	CG1	VAL	264	31.373	8.082	61.372	1.00 22.08	В
	ATOM	1958		VAL	264	29.627	7.398	59.691	1.00 23.20	В
70	ATOM	1959	c	VAL	264	33.425	7.645	59.112	1.00 23.23	
. •										. В
	MOTA	1960	0	VAL	264	33.776	6.482	58.994	1.00 25.35	В
	MOTA	1961	N	ASP	265	34.262	8.625	59.443	1.00 23.36	В
	ATOM	1962	CA	ASP	265	35.683	8.397	59.709	1.00 21.00	В
						-				_

	MOTA	1963	CB	ASP	265	36.528	9.471	59.011	1.00 17.94	В
	ATOM	1964	CG	ASP	265	38.024	9.311	59.258	1.00 18.29	В
	MOTA	1965		ASP	265	38.429	8.960	60.384	1.00 17.19	В
5	MOTA MOTA	1966 1967	C C	ASP	265 265	38.806 35.840	9.554	58.322	1.00 15.43	В
-	MOTA	1968	Ö	ASP ASP	265	36.208	8.501 9.550	61.230 61.758	1.00 21.25 1.00 22.30	B B
	MOTA	1969	N	LEU	266	35.552	7.406	61.928	1.00 22.30	B
	ATOM	1970	CA	LEU	266	35.636	7.387	63.387	1.00 19.48	В
	ATOM	1971	CB	LEU	266	35.269	5.991	63.913	1.00 17.26	В
10	MOTA	1972	CG	LEU	266	33.871	5.454	63.567	1.00 18.72	В
	ATOM	1973	CD1	LEU	266	33.752	4.005	64.042	1.00 15.87	В
	MOTA	1974	CD2	LEU	266	32.792	6.332	64.207	1.00 17.11	₿
	MOTA	1975	С	LEU	266	37.008		63.936	1.00 17.95	В
15	MOTA	1976	0	LEU	266	37.982	7.938	63.198	1.00 16.50	В
13	ATOM	1977	N	ALA	267	37.053	8.062	65.243	1.00 16.22	В
	ATOM	1978	CA	ALA	267	38.284	8.458	65.920	1.00 17.36	В
	ATOM ATOM	1979 1980	CB	ALA ALA	267 267	37.957 39.112	9.144 7.202	67.244 66.183	1.00 13.49 1.00 18.67	. В
	ATOM	1981	ŏ	ALA	267	38.561	6.119	66.320	1.00 18.45	B
20	MOTA	1982	N	GLY	. 268	40.430	7.357	66.249	1.00 18.66	В
	ATOM	1983	CA	GLY	268	41.291	6.226	66.507	1.00 20.51	В
	MOTA	1984	Ċ	GLY	268	40.738	5.336	67.604	1.00 22.52	В
	MOTA	1985	0	GLY	268	40.123	5.815	68.545	1.00 22.16	В
25	MOTA	1986	N	SER	269	40.974	4.033	67.483	1.00 23.43	В
25	MOTA	1987	CA	SER	269	40.471	3.075	68.461	1.00 25.19	, B
	MOTA	1988	СВ	SER	269	40.083	1.796	67.750	1.00 24.66	. В
	MOTA	1989	OG	SER	269	41.131	1.412	66.883	1.00 25.58	В
	MOTA MOTA	1990 1991	C	SER	269	41.446	2.739	69.584	1.00 26.21	В
30	ATOM	1992	N	SER GLU	269 270	41.100 42.657	1.996 3.286	70.493 69.520	1.00 24.37 1.00 28.26	В
-	ATOM	1993	CA	GLU	270	43.664	3.029	70.546	1.00 28.28	B B
	ATOM	1994	СВ	GLU	270	45.031	3.589	70.118	1.00 31.04	В
	MOTA	1995	CG	GLU	270	45.140	5.113	70.033	1.00 28.41	В
~-	MOTA	1996	CD	GLU	270	44.679	5.680	68.701	1.00 28.74	В
35	ATOM	1997	OE1	GLU	270	44.875	6.895	68.471	1.00 30.30	В
	MOTA	1998		GLU	270	44.129	4.921	67.884	1.00 28.84	В
	ATOM	1999	С	GLU	270	43.262	3.618	71.904	1.00 35.40	В
	MOTA	2000	0	GLU	270	42.847	4.770	71.993	1.00 34.74	В
40	MOTA	2001	N	ASN	271	43.378	2.798	72.950	1.00 40.25	В
70	MOTA MOTA	2002 2003	CA CB	ASN ASN	271 271	43.039 41.581	3.192 3.693	74.324	1.00 44.12	В
	ATOM	2003	CG	ASN	271	40.546	2.600	74.419 74.147	1.00 45.82 1.00 46.03	B B
	ATOM	2005		ASN	271	39.347	2.845	74.224	1.00 45.22	В
	ATOM	2006	ND2	ASN	271	41.011	1.395	73.829	1.00 47.11	В
45	MOTA	2007	С	ASN	271	43.246	2.039	75.307	1.00 45.92	В
	ATOM	2008	0	ASN	271	43.668	0.938	74.922	1.00 46.63	В
	MOTA	2009	N	ASN	287	41.544	11.757	79.480	1.00 56.32	В
	ATOM	2010	CA	ASN	287	40.687	12.175	78.374	1.00 56.59	В
50	MOTA	2011	СВ	ASN	287	41.514	12.914	77.315	1.00 58.79	В
50	ATOM	2012 2013	CG	ASN	287	42.376	14.006	77.912	1.00 60.93	В
	MOTA MOTA	2013		ASN ASN	287 287	43.344	13.729 15.259	78.617 77.637	1.00 62.31	В
	MOTA	.2015	C	ASN	287	42.024 39.995	10.965	77.736	1.00 61.77 1.00 54.81	B B
	ATOM	2016	ŏ	ASN	287	40.651	10.079	77.181	1.00 55.49	В
55	MOTA	2017	N	ILE	288	38.667	10.940	77.811	1.00 50.95	В
	ATOM	2018	CA	ILE	288	37.889	9.838	77.252	1.00 46.25	В
	ATOM	2019	CB	ILE	288		9.250		1.00 48.90	В
	MOTA	2020	CG2	ILE	288	37.713	8.784	79.530	1.00 49.46	В
C O	MOTA	2021		ILE	288	35.903	10.307	78.741	1.00 49.66	В
60	MOTA	2022		ILE	288	34.687	9.730	79.435	1.00 51.96	В
	MOTA	2023	C	ILE	288	37.060	10.259	76.039	1.00 40.91	В
	MOTA	2024	0	ILE	288	36.680	11.423	75.904	1.00 41.77	В
	MOTA MOTA	2025 2026	N CA	ASN ASN	289 289	36.774	9.302 9.582	75.163	1.00 32.95	В
65	MOTA	2027	CB	ASN	289	35.979 36.674	9.045	73.976 72.728.	1.00 26.09 1.00 22.00	B B
	MOTA	2028	CG	ASN	289	36.093	9.612	71.444	1.00 22.00	В
	MOTA	2029		ASN	289	36.819	9.927	70.521	1.00 19.84	В
	MOTA	2030	ND2		289	34.774	9.725	71.382	1.00 17.42	В
70	MOTA	2031	С	ASN	289	34.624	8.927	74.154	1.00 22.64	В
70	MOTA	2032	0	ASN	289	34.394	7.805	73.718	1.00 22.38	В
	MOTA	2033	N	GLN	290	33.726	9.652	74.806	1.00 20.05	В
	MOTA	2034	CA	GLN	290	32.386	9.166	75.085	1.00 18.94	В
	MOTA	2035	СВ	GLN	290	31.542	10.299	75.659	1.00 20.27	В

	MOTA	2036	CG	GLN	290	30.18	0 9.847	76.124	1.00 20.13	В
	ATOM	2037	CD	GLN	290	30.27			1.00 20.41	В
	ATOM	2038		GLN	290	29.31			1.00 22.39	В
5	ATOM	2039		GLN	290	31.43			1.00 20.99	В
J	MOTA	2040	Ç	GLN	290	31.69			1.00 18.42	В
	MOTA	2041	0	GLN	290	30.94			1.00 15.37	В
	MOTA	2042	N	SER	291	31.80	8 9.088	72.704	1.00 19.89	В
	ATOM	2043	CA	SER	291	31.13	9 8.540	71.526	1.00 21.11	В
	ATOM	2044	CB	SER	291	31.16			1.00 22.02	В
10	ATOM	2045	OG	SER	291	30.12			1.00 23.09	В
10										
	ATOM	2046	,C	SER	291	31.79			1.00 22.87	В
	ATOM	2047	0	SER	291	31.05			1.00 24.87	В
	ATOM	2048	N	LEU	292	33.07	4 7.107	71.187	1.00 21.56	В
_ ·	MOTA	2049	CA	LEU	292	33.74	1 5.878	70.812	1.00 21.17	В
15	MOTA	2050	СВ	LEU	292	35.24	7 6.097	70.826	1.00 18.31	В
	ATOM	2051	CG	LEU	292	36.07			1.00 18.27	В
	ATOM	2052	CD1		292	35.65			1.00 13.66	B
	ATOM	2053		LEU	292	37.54			1.00 17.97	
										В
20	ATOM	2054	Ç	LEU	292	33.34			1.00 21.64	В
20	MOTA	2055	0	LEU	292	32.91			1.00 19.24	, В
	ATOM	2056	N	LEU	293	33.48	1 5.100	73.098	1.00 22.14	В
	MOTA	2057	CA	LEU	293	33.14	1 4.172	74.158	1.00 22.23	В
	MOTA	2058	CB	LEU	293	33.37	4 4.841	75.513	1.00 22.95	В.
	ATOM	2059	CG	LEU	293	34.47			1.00 25.37	В
25	ATOM	2060		LEU	293	35.68			1.00 25.32	В
	ATOM	2061		LEU	293	34.85			1.00 26.42	В
	ATOM									
		2062	C	LEU	293	31.68			1.00 24.05	В
	ATOM	2063	0	LEU	293	31.37			1.00 27.12	В
20	ATOM	2064	N	THR	294	30.80			1.00 23.43	. В
30	MOTA	2065	CA	THR	294	29.39	6 4.293	73.534	1.00 22.37	В
	MOTA	2066	CB	THR	294	28.55	4 5.580	73.487	1.00 22.35	В
	MOTA	2067	OG1	THR	294	28.70	6 6.277	74.734	1.00 19.68	В
	ATOM	2068	CG2	THR	294	27.09			1.00 19.85	В
	ATOM	2069	c	THR	294	29.14			1.00 23.90	В
35·	ATOM	2070		THR	294	28.27			1.00 26.74	
55			0							В
	MOTA	2071	N	LEU	295	29.93			1.00 24.08	В
	ATOM	2072	CA	LEU	295	29.81			1.00 24.42	В
	ATOM	2073	CB	LEU	295	30.82	2 3.332	69.004	1.00 22.92	В
	ATOM	2074	CG	LEU	295	30.94	0 2.449	67.760	1.00 22.72	В
40	ATOM	2075	CD1	LEU	295	29.64	7 2.481	66.975	1.00 20.45	В
	MOTA	2076		LEU	295	32.09			1.00 22.47	В
	MOTA	2077	C	LEU	295	30.06			1.00 26.15	В
	ATOM	2078	ŏ	LEU	295	29.36			1.00 28.14	В
		2079								
45	ATOM		N	GLY	296	31.07			1.00 26.16	В
40	ATOM	2080	CA	GLY	296	31.39			1.00 25.55	В
	MOTA	2081	C	GLY	296	30.30			1.00 25.59	В
	ATOM	2082	Ο.	GLY	296	29.89	8 -2.059	72.134	1.00 26.11	В
	ATOM	2083	N	ARG	297	29.81	7 -0.162	73.346	1.00 22.71	В
	ATOM	2084	CA	ARG	297	28.76	0 -0.660	74.217	1.00 22.15	В
50	ATOM	2085	CB	ARG	297	28.52	8 0.306	75.372	1.00 19.27	В
	ATOM	2086	CG	ARG	297	29.71			1.00 20.29	В
	MOTA	2087	CD	ARG	297	29.45			1.00 22.43	В
	ATOM	2088.	NE	ARG	297	30.63			1.00 26.34	
		2089		ARG						В
55	MOTA		CZ		297	31.22			1.00 24.22	В
22	MOTA	2090	NH1		297	30.72			1.00 23.11	В
	MOTA	2091	NH2	ARG	297	32.30			1.00 18.73	В
	MOTA	2092	С	ARG	297	27.44	9 -0.876	73.452	1.00 21.70	В
	MOTA	2093	0	ARG	297	26.63	4 -1.674	73.844	1.00 20.12	В.
	MOTA	2094	N	VAL	298	27.25			1.00 23.14	В
60 -	ATOM	2095	CA	VAL	298	26.04		71.558	1.00 23.54	В
••	MOTA	2096	CB	VAL	298	25.84		70.613	1.00 22.84	
										В
	MOTA	2097		VAL	298	24.74		69.582	1.00 18.86	В
	MOTA	2098		VAL	298	25.47		71.432	1.00 19.90	В
65	MOTA	2099	С	VAL	298	26.15		70.739	1.00 25.65	В
65	MOTA	2100	0	VAL	298	25.19	2 -2.325	70.643	1.00 27.92	В
	MOTA	2101	N	ILE	299	27.31		70.147	1.00 25.96	В
	ATOM	2102	CA	ILE	299	27.51		69.354	1.00 27.94	В
	ATOM	2103	CB	ILE	299	28.88		68.649	1.00 26.11	В
	MOTA	2104		ILE	299	29.18		68.053		
70									1.00 24.74	В
/ 0	MOTA	2105		ILE	299	28.86		67.550	1.00 26.37	В
	MOTA	2106		ILE	299	30.19		66.889	1.00 28.12	В
	ATOM	2107	C .	ILE	299	27.41		70.235	1.00 29.09	В
	MOTA	2108	0	ILE	299	26.95	8 -5.284	69.791	1.00 28.96	В

	ATOM	2109	N	THR	300	27.829	-4.112	71.490	1.00 29.82	В
	MOTA	2110	CA	THR	300	27.771	-5.213	72.440	1.00 30.01	В
	ATOM	2111	CB	THR	300	28.561	-4.877	73.706	1.00 29.27	В
	ATOM	2112		THR	300	29.960				
5							-4.842	73.392	1.00 30.68	В
ب	MOTA	2113	CG2		300	28.299	-5.900	74.796	1.00 28.12	В
	MOTA	2114	С	THR	300	26.330	-5.517	72.821	1.00 32.39	В
	MOTA	2115	0	THR	300	25.927	-6.675	72.902	1.00 33.67	В
	MOTA	2116	N	ALA	301	25.552	-4.467	73.044	1.00 32.46	В
	ATOM	2117	CA	ALA	301	24.157		73.414	1.00 34.19	В
10	ATOM	2118	CB	ALA	301	23.584	-3.305	73.863	1.00 32.83	В
10										
	ATOM	2119	C	ALA	301	23.353	-5.182	72.238	1.00 35.75	В
	MOTA	2120	0	ALA	301	22.348	-5.842	72.425	1.00 37.02	В
	MOTA	2121	N	LEU	302	23.812	-4.899	71,024	1.00 36.43	В
	ATOM	2122	CA	LEU	302	23.132	-5.352	69.817	1.00 38.14	В
15	ATOM	2123	CB	LEU	302	23.549	-4.488	68.622	1.00 38.00	В
	ATOM	2124	CG	LEU	302	22.492	-3.555	68.031	1.00 39.25	В
	ATOM	2125		LEU	302	21.823	-2.753	69.128	1.00 39.09	. В
					302			67.016		
	ATOM	2126		LEU		23.149	-2.630		1.00 38.56	В
20	MOTA	2127	Ç	LEU	302	23.428	-6.812	69.514	1.00 39.23	B
20	MOTA	2128	0	LEU	302	22.520	-7.594	69.249	1.00 39.50	В
	ATOM	2129	N	VAL	303	24.709	-7.163	69.552	1.00 40.87	В
	ATOM.	2130	CA	VAL	303	25.161	-8.521	69.287	1.00 42.58	В
	MOTA	2131	CB	VAL	303	26.706	-8.605	69.331	1.00 42.52	В
	ATOM	2132		VAL	303	27.155	-10.051	69.270	1.00 43.58	В
25	ATOM	2133		VAL	303	27.301	-7.824	68.167		
LJ									1.00 42.05	В
	ATOM	2134	C	VAL	303	24.579	-9.496	70.306	1.00 44.19	. В
	ATOM	2135		VAL	303		-10.538	69.941	1.00 45.04	В
	MOTA	2136	N	GLU	304	24.685	-9.145	71.584	1.00 45.93	В
	ATOM	2137	CA	GLU	304	24.169	-9.973	72.667	1.00 48.10	В
30	MOTA	2138	CB	GLU	304	24.792	-9.541	73.998	1.00 47.26	В
	MOTA	2139	CG	GLU	304	26.305	-9.707	74.041	1.00 46.33	В
		2140	CD	GLU	304	26.901	-9.334	75.382	1.00 46.65	В
		2141								
	MOTA			GLU	304	28.139	-9.410	75.519	1.00 44.41	В
25	MOTA	2142		GLU	304	26.135	-8.968	76.302	1.00 47.42	В
35	MOTA	2143	С	GLU	304	22.649	-9.885	72.753	1.00 49.92	В.
	ATOM	2144	0	GLU	304	22.031	-10.492	73.612	1.00 50.02	В
	ATOM	2145	N	ARG	305	22.061	-9.116	71.844	1.00 52.91	В
	ATOM	2146	CA	ARG	305	20.614	-8.941	71.787	1.00 56.32	В
	ATOM	2147	CB	ARG	305		-10.251	71.357	1.00 58.76	В
40	ATOM	2148	CG	ARG	305					
70							-10.652	69.934	1.00 63.36	В
	MOTA	2149	CD	ARG	305		-11.856	69.475	1.00 68.00	В
	ATOM	2150	NE	ARG	305		-12.133	68.057	1.00 71.78	В
	MOTA	2151	CZ	ARG	305	19.306	-11.344	67.068	1.00 73.93	В
	ATOM	2152	NH1	ARG	305	18.650	-10.222	67.339	1.00 74.69	B
45	ATOM	2153	NH2	ARG	305	19.554	-11.675	65.807	1.00 75.22	В
	MOTA	2154	С	ARG	305	19.981	-8.443	73.082	1.00 56.68	В
	ATOM	2155	ō	ARG	305	18.809	-8.699	73.340	1.00 56.68	В
	MOTA	2156	N	THR	306	20.757	-7.728	73.892		
								73.632	1.00 57.02	В
50	MOTA	2157	CA	THR	306	20.248	-7.185	75.146	1.00 56.82	В
J U	MOTA	2158	CB	THR	306	21.347	-6.426	75.912	1.00 56.33	В
	MOTA	2159	OG1		306	22.482	-7.281	76.095	1.00 56.76	₿
	ATOM	2160	CG2	THR	306	20.836	-5.975	77.272	1.00 56.64	В
	ATOM	2161	С	THR	306	19.122	-6.213	74.812	1.00 57.35	В
	ATOM	2162	0	THR	306	19.239	-5.421	73.881	1.00 58.12	В
55	ATOM	2163	N	PRO	307	18.011	-6.268	75.564	1.00 57.68	В
	ATOM	2164	CD	PRO ·		17.750	-7.184	76.688	1.00 58.36	
										В
	ATOM	2165	CA	PRO	307	16.861	-5.384	75.336	1.00 57.69	В
	MOTA	2166	CB	PRO	307	15.959	-5.682	76.533	1.00 57.98	В
~	ATOM	2167	CG	PRO	307	16.241	-7.125	76.803	1.00 58.68	· В
60	MOTA	2168	C	PRO	307	17.218	-3.898	75.237	1.00 56.99	В
	MOTA	2169	0	PRO	307	16.684	-3.187	74.386	1.00 57.64	В
	ATOM	2170	N	HIS	308	18.120	-3.439	76.105	1.00 55.27	В
	ATOM	2171	CA	HIS	308	18.539	-2.034	76.123		
		2172							1.00 53.51	В
65	MOTA		CB	HIS	308	18.749	-1.565	77.567	1.00 55.71	B '
UJ	MOTA	2173	CG	HIS	308	19.227	-0.150	77.677	1.00 58.12	В
	MOTA	2174		HIS	308	20.385	0.367	78.155	1.00 59.12	В
	MOTA	2175	ND1	HIS	308	18.475	0.925	77.252	1.00 58.97	В
	MOTA	2176	CE1		308	19.148	2.043	77.464	1.00 58.91	В
	ATOM	2177	NE2		308	20.310	1.732	78.012	1.00 59.24	В
70	ATOM	2178	C	HIS	308	19.813	-1.749	75.329	1.00 50.82	В
. •	ATOM	2179	ŏ	HIS	308					
						20.793	-2.472	75.433	1.00 50.26	В
	MOTA	2180	N	VAL	309	19.780	-0.671	74.551	1.00 47.79	В
	MOTA	2181	CA	VAL	309	20.921	-0.239	73.743	1.00 44.18	В

	ATOM	2182	СВ	VAL	309	20.619	-0.355	72.233	1.00 44.37	
	MOTA	2183		VAL	309	21.876	-0.067	71.427	1.00 43.69	B B
	MOTA	2184	CG2		309	20.076	-1.737	71.912	1.00 43.59	В
	MOTA	2185	C	VAL	309	21.188	1.234	74.075	1.00 41.50	В
5	ATOM	2186	ŏ	VAL	309	20.368	2.091	73.788	1.00 41.50	В
•	ATOM	2187	N	PRO	310	22.351	1.535	74.675	1.00 38.54	В
	ATOM	2188	CD	PRO	310	23.440	0.586	74.968	1.00 37.32	В
	ATOM	2189	CA	PRO	310	22.736	2.898	75.058	1.00 37.55	В
	ATOM	2190	CB	PRO	310	23.983	2.669	75.909	1.00 36.77	В
10	MOTA	2191	CG	PRO	310	24.614	1.502	75.238	1.00 36.14	В
	MOTA	2192	. c	PRO	310	22.977	3.898	73.917	1.00 36.95	В
	MOTA	2193	ō	PRO	310	24.042	4.493	73.827	1.00 36.57	В
	MOTA	2194	N	TYR	311	21.972	4.076	73.061	1.00 36.05	В
	MOTA	2195	CA	TYR	311	22.047	5.012	71.940	1.00 34.95	В
15	ATOM	2196	CB	TYR	311	20.778	4.949	71.085	1.00 35.41	В
	MOTA	2197	CG	TYR	311	20.603	3.711	70.245	1.00 36.70	В
	MOTA	2198		TYR	311	21.603	3.289	69.374	1.00 35.89	В
	MOTA	2199		TYR	311	21.433	2.161	68.578	1.00 36.91	В
20	MOTA	2200	CD2	TYR	311	19.416	2.973	70.300	1.00 36.75	В
20	MOTA	2201	CE2		311	19.234	1.844	69.508	1.00 36.61	В
	MOTA	2202	CZ	TYR	311	20.247	1.442	68.651	1.00 36.85	В
	ATOM	2203	ОН	TYR	311	20.086	0.312	67.882	1.00 35.56	В,
	ATOM	2204	C	TYR	311	22.217	6.462	72.402	1.00 35.12	В
25	ATOM	2205	0	TYR	311	23.038	7.186	71.868	1.00 34.13	· B
LJ	MOTA	2206	N	ARG	312	21.422	6.868	73.392	1.00 34.48	В
	MOTA ATOM	2207 2208	CA CB	ARG	312 312	21.444 20.160	8.237	73.906	1.00 34.28	В
	ATOM	2209	CG	ARG	312	18.882	8.523 8.227	74.690 73.935	1.00 35.83 1.00 41.17	В
	ATOM	2210	CD	ARG	312	17.732	8.007	74.897	1.00 41.17	B B
30	ATOM	2211	NE	ARG	312	16.596	7.341	74.263	1.00 44.62	В
	ATOM	2212	cz	ARG	312	15.608	6.747	74.926	1.00 51.08	В
	ATOM	2213		ARG	312	15.610	6.732	76.254	1.00 50.32	В
	MOTA	2214	NH2		312	14.618	6.163	74.259	1.00 51.58	В
	MOTA	2215	C	ARG	312	22.638	8.593	74.787	1.00 33.03	В
35 [.]	ATOM .	. 2216	0	ARG	312	22.701	9.699	75.317	1.00 34.26	В
	ATOM	2217	N	GLU	313	23.581	7.669	74.953	1.00 29.69	В
	MOTA	2218	CA	GLU	313	24.735	7.947	75.799	1.00 25.30	В
	MOTA	2219	CB	GLU	313	25.200	6.655	76.481	1.00 24.49	В
40	MOTA	2220	CG	GLU	313	24.278	6.242	77.634	1.00 25.08	В
40	MOTA	2221	CD	GLU	313	24.677	4.946	78.327	1.00 23.59	В
	MOTA	2222		GLU	313	25.883	4.722	78.553	1.00 23.79	В
	MOTA	2223	OE2		313	23.775	4.156	78.665	1.00 23.87	В
	MOTA	2224	Ç	GLU	313	25.898	8.646	75.089	1.00 23.89	В
45	MOTA	2225	0	GLU	313	26.963	8.806	75.659	1.00 23.12	В
40	MOTA	2226	N	SER	314	25.680	9.068	73.843	1.00 21.70	В
	MOTA MOTA	2227 2228	CA	SER	314	26.714	9.766	73.080	1.00 21.61	В
	ATOM	2229	CB OG	SER SER	314	27.800	8.796	72.622	1.00 19.78	В
	ATOM	2230	C.	SER	314 314	27.401 26.124	8.118 10.466	71.442	1.00 17.85 1.00 23.50	В
50	ATOM	2231	ŏ	SER	314	25.047	10.105	71.388	1.00 23.30	B B
	ATOM	2232	N	LYS	315	26.840	11.462	71.348	1.00 23.77	В
	ATOM	2233	CA	LYS	315	26.367	12.204	70.186	1.00 24.56	В
	MOTA	2234	СВ	LYS	315	27.216	13.462	69.963	1.00 24.98	В
	ATOM	2235	CG	LYS	315	27.295	14.394	71.165	1.00 25.63	В
55	MOTA	2236	CD	LYS	315	25.926	14.862	71.607	1.00 25.73	В
	MOTA	2237	CE	LYS	315	26.034	15.834	72.774	1.00 26.31	В
	MOTA	2238	NZ	LYS	315	26.660	17.123	72.353	1.00 30.29	В
	ATOM	2239	С	LYS	315	26.416	11.335	68.939	1.00 24.22	В.
۲۵	MOTA	2240	0	LYS	315	25.498	11.338	68.138	1.00 25.98	В
60	MOTA	2241	N	LEU	316	27.503	10.591	68.787	1.00 23.22	В
	MOTA	2242	CA	LEU	316	27.674	9.719	67.636	1.00 24.18	В
	MOTA	2243	СВ	LEU	316	29.039	9.022	67.711	1.00 24.13	В
	MOTA	2244	CG	LEU	316	29.451	8.205	66.488	1.00 23.55	В
65	MOTA	2245	CD1		316	29.850	9.149	65.370	1.00 25.34	В
U)	MOTA	2246	CD2		316	30.609	7.299	66.840	1.00 22.84	В
	MOTA	2247	C	LEU	316	26.567	8.664	67.506	1.00 23.18	В
	MOTA	2248	0	LEU	316	25.892	8.590	66.480	1.00 22.77	В
	ATOM	2249	N	THR	317	26.369	7.855	68.543	1.00 22.09	В
70	MOTA MOTA	2250 2251	CA	THR	317	25.346	6.817	68.470	1.00 22.50	В
	MOTA	2252	CB OG1	THR	317 317	25.459 25.198	5.809	69.651	1.00 20.87	В
	MOTA	2253	CG2		317	25.198 26.848	6.472 5.192	70.892 69.682	1.00 19.26 1.00 20.16	В
	MOTA	2254	C	THR	317	23.923	7.367	68.394	1.00 20.16	B B
			-			,		33.334	00 23.33	D

	MOTA	2255	0	THR	317	23.025	6.684	67.929	1.00 23.95	В
	MOTA	2256	N	ARG	318	23.723	8.606	68.836	1.00 23.82	В
	ATOM	2257	CA	ARG	318	22.402	9.225	68.764	1.00 25.01	В
	ATOM	2258	СB	ARG	318	22.317	10.426	69.705	1.00 28.63	В
5				ARG						
,	MOTA	2259	CG		318	21.923	10.065	71.120	1.00 34.53	В
	ATOM	2260	CD	ARG	318	22.260	11.179	72.094	1.00 38.92	₿
	MOTA	2261	NE	ARG	318	21.606	12.436	71.745	1.00 45.13	В
	MOTA	2262	CZ	ARG	318	20.293	12.642	71.792	1.00 47.64	В
	MOTA	2263	NH1	ARG	318	19.479	11.666	72.177	1.00 49.68	В
10	MOTA	2264	NH2		318	19.796	13.826	71.456	1.00 45.41	В
	ATOM	2265	С	ARG	318	22.127	9.674	67.335	1.00 24.81	. B
	ATOM	2266	ŏ	ARG	318	21.015	9.522	66.828	1.00 24.93	В
	MOTA	2267	N	ILE	319			66.684	1.00 22.86	В
15	ATOM	2268	CA	ILE	319	23.001	10.688	65.313	1.00 23.60	В
15	MOTA	2269	CB	ILE	319 .		11.588	64.893	1.00 22.37	В
	MOTA	2270	CG2	ILE	319	24.089	11.947	63.410	1.00 22.84	В
	MOTA	2271	. CG1	ILE	319	24.224	12.861	65.748	1.00 22.76	. В
	ATOM	2272	CD1	ILE	319	25.457	13.738	65.533	1.00 17.34	В
	MOTA	2273	C	ILE	319	22.903	9.532	64.322	1.00 24.40	В
20	ATOM	2274	ŏ	ILE	319	22.144	9.585	63.381	1.00 23.60	В
~~	ATOM	2275	Ŋ	LEU	320	23.688	8.486	64.556		
									1.00 27.00	В
	ATOM .	2276	CA	LEU	320	23.725	7.331	63.664	1.00 28.83	В
	ATOM	2277	CB	LEU	320	25.180	7.037	63.274	1.00 26.75	В
0.5	ATOM	2278	CG	LEU	320	26.035	8.151	62.668	1.00 28.19	В
25	ATOM	2279	CD1	LEU	320	27.479	7.720	62.710	1.00 27.81	В
	MOTA	2280	CD2	LEU	320	25.601	8.459	61.237	1.00 26.81	. в
	MOTA	2281		LEU	320	23.098	6.053	64.220	1.00 30.42	В
	ATOM	2282	ŏ	LEU	320	23.501	4.957	63.841	1.00 31.06	В
	MOTA	.2283	N	GLN	321	22.097	6.188	65.085	1.00 32.73	В
30									1.00 34.42	
50	MOTA	2284	CA	GLN	321	21.457	5.012	65.674		В
	MOTA	2285	CB	GLN	321	20.466	5.419	66.777	1.00 35.23	В
	MOTA	2286	CG	GLN	321	19.195	6.116	66.314	1.00 39.71	В
	MOTA	2287	CD	GLN	321	18.320	6.569	67.488	1.00 42.32	В
~-	MOTA	2288	OE1	GLN	321	17.881	5.755	68.298	1.00 42.09	В
35	ATOM	2289	NE2	GLN	·321	18.069	7.877	67.577	1.00 44.14	В
	ATOM	2290	С	GLN	321	20.758	4.102	64.663	1.00 33.44	В
	ATOM	2291	ō	GLN	321	20.677	2.901	64.868	1.00 34.48	В
	MOTA	2292	N	ASP	322	20.261	4.666			
								63.569	1.00 32.24	В
40	MOTA	2293	CA	ASP	322	19.583	3.839	62.575	1.00 33.02	В
40	MOTA	2294	CB	ASP	322	18.780	4.693	61.595	1.00 32.22	В
	MOTA	2295	CG	ASP	322	17.790	3.871	60.783	1.00 32.38	В
	ATOM	2296	OD1	ASP	322	17.716	4.061	59.548	1.00 32.08	В
	ATOM	2297	OD2	ASP	322	17.074	3.045	61.382	1.00 30.54	В
	ATOM	2298	С	ASP	322	20.598	3.011	61.794	1.00 32.49	В
45	MOTA	2299	0	ASP	322	20.228	2.175	60.988	1.00 32.45	В
	ATOM	2300	N	SER	323	21.880	3.274	62.030	1.00 32.77	В
	ATOM	2301	CA	SER	323	22.951	2.547	61.361	1.00 30.97	В
	ATOM	2302	CB	SER	323	24.122	3.480	61.067		
									1.00 28.95	В
50	MOTA	2303	OG	SER	323	23.837	4.320	59.959	1.00 27.41	В
20	MOTA	2304	C	SER	323	23.416	1.374	62.224	1.00 30.75	В
	ATOM	2305	0	SER	323	24.171	0.517	61.783	1.00 29.17	В
	MOTA	2306	N	LEU	324	22.966	1.352	63.470	1.00 30.45	В
	ATOM	2307	CA	LEU	324	23.326	0.270	64.363	1.00 31.28	В
	MOTA	2308	CB	LEU	324	24.046	0.809	65.606	1.00 31.28	В
55	ATOM	2309	CG	LEU	324	25.476	1.353	65.463	1.00 32.14	В
	ATOM	2310		LEU	324	26.308	0.424	64.587	1.00 33.04	В
	MOTA	2311		LEU	324	25.436	2.739	64.862		
									1.00 34.26	В
	MOTA	2312	C	LEU	324	22.081	-0.511	64.771	1.00 31.54	В
40	MOTA	2313	0	LEU	324	21.468	-0.235	65.785	1.00 31.30	В
60	MOTA	2314	N	GLY	325	21.715	-1.490	63.950	1.00 33.73	В
	MOTA	2315	CA	GLY	325	20.554	-2.311	64.249	1.00 33.79	В
	ATOM	2316	C	GLY	325	19.244	-1.636	63.901	1.00 33.20	В
	ATOM	2317	0	GLY	325	18.218	-1.905	64.517	1.00 33.16	В
	ATOM	2318	N	GLY	326	19.286	-0.754	62.909	1.00 32.43	В
65	MOTA	2319	CA	GLY	326	18.090	-0.048	62.499	1.00 33.13	В
	MOTA	2320				17.704				
			C	GLY	326		-0.420	61.088	1.00 34.86	В
	ATOM	2321	0	GLY	326	17.905	-1.541	60.680	1.00 34.93	В
	MOTA	2322	N	ARG	327	17.157	0.535	60.343	1.00 37.13	В
70	ATOM	2323	CA	ARG	327	16.748	0.278	58.974	1.00 38.94	В
70	ATOM	2324	CB	ARG	327	15.327	0.784	58.753	1.00 43.05	В
	MOTA	2325	CG	ARG	327	14.278	0.034	59.559	1.00 49.59	В
	ATOM	2326	CD	ARG	327	12.872	0.464	59.159	1.00 54.64	В
	MOTA	2327	NE	ARG	327	12.071	-0.657	58.665	1.00 60.40	В
		- -						32.000		_

	MOTA	2328	cz	ARG	327	12.358	-1.380	57.583	1.00 62.77	В
	ATOM	2329		ARG	327	13.441	-1.105	56.861	1.00 63.46	В
	ATOM	2330	NH2	ARG	327	11.556	-2.377	57.219	1.00 61.73	В
_	ATOM	2331	С	ARG	327	17.686	0.887	57.934	1.00 38.03	В
5	MOTA	2332	0	ARG	327	17.249	1.289	56.869	1.00 37.61	В
	MOTA	2333	N	THR	328	18.979	0.931	58.252	1.00 36.37	В
	MOTA	2334	CA	THR	328	19.983	1.481	57.345	1.00 35.54	В
	MOTA	2335	CB	THR	328	20.715	2.685	57.989	1.00 34.89	В
	MOTA	2336	OG1	THR	328	19.798	3.762	58.194	1.00 35.66	В
10	ATOM	2337	CG2	THR	328	21.847	3.156	57.096	1.00 33.72	В
	MOTA	2338	· C	THR	328	21.040	0.442	56.974	1.00 34.98	В
	MOTA	2339	0	THR	328	21.630	-0.170	57.848	1.00 36.65	В
	ATOM	2340	N	ARG	329	21.274	0.252	55.678	1.00 33.43	В
	MOTA	2341	CA	ARG	329	22.281	-0.704	55.226	1.00 33.67	В
15	ATOM .	2342	CB	ARG	329	22.354	-0.752	53.696	1.00 35.61	В
	MOTA	2343	CG	ARG	329	23.146	-1.938	53.156	1.00 40.29	В
	MOTA	2344	CD	ARG	329	23.642	-1.691	51.736	1.00 45.76	В
	MOTA	2345	NE	ARG	329	24.253	-2.877	51.133	1.00 51.83	В
20	MOTA	2346	CZ	ARG	329	25.297	-3.540	51.632	1.00 54.83	В
20	ATOM	2347		ARG	329	25.874	-3.148	52.761	1.00 54.64	В
	MOTA	2348		ARG	329	25.772	-4.601	50.991	1.00 56.00	В
	MOTA	2349	C	ARG	329	23.615	-0.218	55.764	1.00 30.92	В.
	MOTA	2350	0	ARG	329	24.034	0.871	55.452	1.00 33.46	В
25	MOTA	2351	N	THR	330	24.277	-1.028	56.573	1.00 28.10	. В
23	ATOM	2352	CA	THR	330	25.541	-0.622	57.156	1.00 26.64	В
	MOTA	2353	CB	THR	330	25.410	-0.524	58.691	1.00 25.12	В
	MOTA	2354	0G1		330	24.526	0.549	59.019	1.00 25.09	В
	MOTA	2355	CG2		330	26.760	-0.291	59.351	1.00 22.76	В
30	ATOM	2356	C	THR	330	26.723	-1.516	56.820	1.00 27.27	В
50	ATOM	2357 2358	0	THR	330	26.602	-2.732	56.748	1.00 27.57	В
	MOTA MOTA	2359	N CA	SER	331	27.868	-0.878 -1.567	56.618	1.00 26.82	В
	MOTA	2360	. CB	SER SER	331 331	29.104 29.442	-1.446	56.308 54.830	1.00 26.67 1.00 26.29	В
	ATOM	2361	OG	SER	331	28.444	-2.072	54.052	1.00 28.29	B B
35		2362	c	SER	331	30.191	-0.907	57.125	1.00 31.25	. в
55	ATOM	2363	ŏ	SER	331	30.210	0.304	57.272	1.00 28.03	В
	ATOM	2364	N	ILE	332	31.086	-1.712	57.677	1.00 24.35	В
	ATOM	2365	CA	ILE.	332	32.179	-1.190	58.472	1.00 20.58	В
	ATOM	2366	СВ	ILE	332	32.119	-1.704	59.917	1.00 16.78	В
40	ATOM	2367		ILE	332	33.367	-1.290	60.656	1.00 15.30	В
:	ATOM	2368		ILE	332	30.849	-1.195	60.605	1.00 14.73	В
	ATOM	2369		ILE	332	30.641	-1.735	62.018	1.00 11.20	В
	ATOM	2370	Ċ	ILE	332	33.484	-1.646	57.855	1.00 22.60	В
	MOTA	2371	ō	ILE	332	33.635	-2.809	57.495	1.00 22.21	В
45	MOTA	2372	N	ILE	333	34.421	-0.718	57.713	1.00 23.08	В
-	ATOM	2373	CA	ILE	333	35.718	-1.046	57.148	1.00 21.26	В
	ATOM	2374	CB	ILE	333	36.096	-0.086	56.011	1.00 20.77	В
	ATOM	2375		ILE	333	37.401	-0.530	55.375	1.00 20.19	В
	ATOM	2376		ILE	333	34.993	-0.065	54.950	1.00 22.76	В
50	MOTA	2377		ILE	333	35.297	0.826	53.738	1.00 19.77	В
	ATOM	2378	С	ILE	333	36.736	-0.927	58.267	1.00 22.44	В
	ATOM	2379	0	ILE	333 .	37.015	0.170	58.740	1.00 25.05	В
	ATOM	2380	N	ALA	334	37.269	-2.061	58.708	1.00 22.25	В
	ATOM	2381	CA	ALA	334	38.252	-2.080	59.783	1.00 21.24	В
55	MOTA	2382	CB	ALA	334	38.088	-3.351	60,605	1.00 21.16	В
	MOTA	2383	С	ALA	334	39.667	-1.998	59.212	1.00 20.54	B
	MOTA	2384	0	ALA	334	40.070	-2.850	58.452	1.00 21.75	В
	MOTA	2385	N	THR	335	40.405	-0.952	59.582	1.00 18.02	В
60	MOTA	2386	CA	THR	335	41.772	-0.771	59.102	1.00 15.52	В
60	MOTA	2387	CB	THR	335	42.052	0.701	58.752	1.00 14.93	В
	MOTA	2388		THR	335	41.551	1.558	59.794	1.00 16.56	В
	MOTA	2389		THR	335	41.394	1.051	57.447	1.00 13.76	В
	MOTA	2390	C	THR	335	42.780	-1.257	60.132	1.00 14.40	В
65	MOTA	2391	0	THR	335	42.586	-1.096	61.340	1.00 13.68	В
UJ	ATOM	2392	N	ILE	336	43.863	-1.849	59.641	1.00 15.75	В
	ATOM	2393	CA	ILE	336	44.893	-2.409	60.506	1.00 16.07	В
	ATOM	2394	CB	ILE	336	44.671	-3.936	60.702	1.00 14.75	В
	MOTA	2395		ILE	336	43.346	-4.185	61.401	1.00 13.27	В
70	ATOM	2396		ILE	336	44.678	-4.662	59.348	1.00 15.22	В
70	MOTA	2397		ILE	336	44.726	-6.215	59.461	1.00 13.20	В
	MOTA	2398	c	ILE	336	46.317	-2.186	59.999	1.00 17.99	В
	MOTA	2399	O -	ILE	336	46.534	-1.816	58.844	1.00 17.06	В
	MOTA	2400	N	SER	337	47.280	-2.407	60.889	1.00 20.83	В

	ATOM	2401	CA	SER	337	48.694	-2.250	60.570	1.00 23.58	В
	ATOM	2402	CB	SER	337	49.399	-1.491	61.685	1.00 22.57	. В
	ATOM	2403	OG	SER	337	50.792	-1.737	61.645	1.00 21.86	В
	MOTA	2404	С	SER	337	49.395	-3.600	60.389	1.00 27.32	В
5	ATOM	2405	ō	SER	337	49.123	-4.548	61.122	1.00 27.36	
										В
	ATOM.	2406	N	PRO	338	50.320	-3.688	59.416	1.00 28.03	В
	MOTA	2407	CD	PRO	338	50.612	-2.678	58.383	1.00 29.38	В
	ATOM	2408	CA	PRO	338	51.063	-4.919	_		
								59.147	1.00 30.56	В
••	MOTA	2409	CB	PRO	338	51.485	-4.743	57.698	1.00 29.47	В
10	MOTA	2410	CG	PRO	338	51.804	-3.283	57.657	1.00 28.25	В
	MOTA	2411	C	PRO	338	52.274	-5.047	60.074	1.00 31.99	В
	ATOM	2412	0	PRO	338	52.903	-6.083	60.131	1.00 32.55	В
	ATOM	2413	N	ALA	339	52.586	-3.972	60.790	1.00 33.15	В
	MOTA	2414	CA	ALA	339	53.732	-3.955	61.690	1.00 34.44	В
15										
13	MOTA	2415	CB	ALA	339	54.051	-2.518	62.109	1.00 35.58	В
	ATOM	2416	С	ALA	339	53.505	-4.816	62.918	1.00 35.05	В
	ATOM	2417	0	ALA	339	52.391	-4.956	63.386	1.00 35.58	В
				SER	340	54.585				
	MOTA	2418	N				-5.380	63.447	1.00 36.34	В
-	ATOM	2419	ÇA	SER	340	54.479	-6.236	64.615	1.00 36.42	В
20	ATOM	2420	CB	SER	340	55.694	-7.162	64.717	1.00 36.55	В
	ATOM	2421	OG	SER	340	56.891	-6.431	64.909	1.00 37.23	В
	MOTA	2422	С	SER	340	54.324	-5.457	65.914	1.00 36.18	В
	ATOM	2423	0	SER	340	53.769	-5.969	66.871	1.00 36.17	В
	ATOM	2424	N	LEU	341	54.803	-4.220	65.957	1.00 36.13	В
25										
25	MOTA	2425	CA	LEU	341	54.664	-3.453	67.190	1.00 38.21	В
	MOTA	2426	CB	LEU	341	55.663	-2.296	67.239	1.00 40.75	. В
	ATOM	2427	CG	LEU	341	55.293	-1.011	66.500	1.00 44.27	В
	MOTA	2428		LEU	341	56.054	0.160	67.121	1.00 44.94	В
	MOTA	2429	CD2	LEU	341	55.597	-1.158	65.011	1.00 45.97	В
30	MOTA	2430	С	LEU	341	53.244	-2.912	67.337	1.00 36.82	В
	MOTA	2431	ŏ	LEU	341		-2.185		1.00 37.65	
						52.944		68.259		В
	MOTA	2432	N	ASN	342	52.376	-3.288	66.408	1.00 36.59	В
	ATOM	2433	CA	ASN	342	50.983	-2.856	66.416	1.00 35.71	В
	ATOM	2434	CB	ASN	342	50.636	-2.219	65.071		
35										B
33	MOTA	2435	CG	ASN	342	51.343	-0.903	64.865	1.00 34.11	В
	ATOM	2436	OD1	ASN	342	51.904	-0.649	63.808	1.00 32.85	В
	MOTA	2437		ASN	342	51.315	-0.052	65.888	1.00 32.94	В
	ATOM	2438	С	ASN	342	50.084	-4.048	66.661	1.00 35.91	В
	MOTA	2439	0	ASN	342	48.860	-3.958	66.561	1.00 37.26	В
40	MOTA	2440	N	LEU	343	50.720	-5.164	66.993	1.00 34.56	B
	ATOM	2441	CA	LEU	343	50.033	-6.419	67.244	1.00 32.49	В
	ATOM	2442	CB	LEU	343	51.019	-7.433	67.B36	1.00 31.23	В
	ATOM	2443	CG	LEÙ	343	50.546	-8.858	68.135	1.00 31.25	В
15	ATOM	2444		LEU	343	50.001	-8.944	69.548	1.00 32.82	В
45	ATOM	2445	CD2	LEU	343	49.504	-9.286	67.101	1.00 30.64	В
	MOTA	2446	C	LEU	343	48.817	-6.295	68.140	1.00 30.37	В
	ATOM	2447	0	LEU	343	47.714	-6.608	67.732		
									1.00 29.24	В
	MOTA	2448	N	GLU	344	49.023	-5.831	69.364	1.00 30.64	В
	ATOM	2449	CA	GLU	344	47.922	-5.710	70.307	1.00 32.19	В
50	MOTA	2450	CB	GLU	344	48.442	-5.121	71.619	1.00 34.78	В
	ATOM	2451	CG	GLU	344	47.460	-5.189			
								72.761	1.00 42.18	В
	MOTA	2452	CD	GLU	344	48.107	-4.861	74.099	1.00 47.80	В
	ATOM	2453	OE1	GLU	344	48.743	-3.785	74.209	1.00 48.41	В
	ATOM	2454	OE2	GLU	344	47.982	-5.686	75.036	1.00 49.00	В
55										
"	MOTA	2455	С	GLU	344	46.736	-4.899	69.760	1.00 30.46	, в
	ATOM	2456	0	GLU	344	45.600	-5.355	69.802	1.00 29.53	В
	MOTA	2457	N	GLU	345	46.991	-3.707	69.234	1.00 29.30	В
										_
	MOTA	2458	CA	GLU	345	45.901	-2.891	68.703	1.00 29.30	В
	MOTA	2459	CB	GLU	345	46.393	-1.477	68.349	1.00 29.27	В
60	MOTA	2460	CG	GLU	345	46.618	-0.581	69.565	1.00 29.72	В
	ATOM	2461	CD	GLU	345	45.337				
							-0.285	70.330	1.00 30.47	В
	MOTA	2462		GLU	345	45.429	0.193	71.482	1.00 33.09	В
	MOTA	2463	OE2	GLU	345	44.241	-0.521	69.786	1.00 30:71	В
	ATOM	2464	c	GLU	345	45.277	-3.556	67.476	_	
65									1.00 27.38	. В
UJ	MOTA	2465	0	GLU	345	44.082	-3.423	67.233	1.00 28.53	В
	ATOM	2466	N	THR	346	46.084	-4.283	66.711	1.00 24.59	В
	ATOM	2467	CA	THR	346	45.576	-4.979			
								65.530	1.00 23.55	В
	ATOM	2468	CB	THR	346	46.717	-5.588	64.721	1.00 22.82	В
	ATOM	2469	OG1	THR	346	47.503	-4.534	64.147	1.00 24.62	В
70	MOTA	2470		THR	346	46.173	-6.473	63.618	1.00 23.82	В
	ATOM	2471	C	THR	346	44.597	-6.083	65.937	1.00 22.61	В
	MOTA	2472	0	THR	346	43.617	~6.343	65.252	1.00 22.38	В
	ATOM	2473	N	LEU	347	44.873	-6.732	67.062	1.00 23.16	В
								3	23.10	

	MOTA	2474	CA	LEU	347	44.002	-7.790	67.561	1.00 23.19	В
	MOTA	2475	CB	LEU	347	44.678	-8.568	68.696	1.00 21.66	B
	MOTA	2476			347					
			CG	LEU		45.955	-9.346	68.374	1.00 22.14	В
-	ATOM	2477	CD1	LEU	347	46.393	-10.118	69.613	1.00 20.42	В
5	MOTA	2478	CD2	LEU	347	45.718	-10.293	67.210	1.00 22.20	В
	ATOM	2479	C	LEU	347	42.679	-7.203	68.063	1.00 23.83	В
	ATOM'	2480	õ	LEU	347	41.617	-7.712	67.732	1.00 25.14	В
	MOTA	2481	N	SER	348	42.743	-6.135	68.854	1.00 21.92	В
• •	MOTA	2482	CA	SER	348	41.518	-5.530	69.368	1.00 23.12	В
10	MOTA	2483	CB	SER	348	41.839	-4.306	70.215	1.00 21.23	В
	MOTA	2484	· OG	SER	348	42.491	-4.707	71.402	1.00 27.13	В
	ATOM	2485	c	SER	348	40.582	-5.144	68.238	1.00 22.86	В
•	MOTA	2486	0	SER	348	39.384	-5.348	68.331	1.00 22.12	В
	MOTA	2487	N	THR	349	41.156	-4.596	67.172	1.00 23.05	В
15	MOTA	2488	CA	THR	349	40.391	-4.186	66.005	1.00 25.38	В
	MOTA	2489	CB	THR	349	41.309	-3.483	64.988	1.00 25.69	В
•	MOTA	2490		THR	349	41.656	-2.185	65.495	1.00 28.94	В
	ATOM	2491	CG2		349	40.627	-3.334	63.639	1.00 26.37	В
^^	MOTA	2492	Ç	THR	349	39.714	-5.387	65.344	1.00 27.04	В
20	ATOM	2493	0	THR	349	38.502	-5.396	65.164	1.00 25.10	В
	ATOM	2494	N	LEU	350	40.505	-6.399	64.988	1.00 29.73	В
	ATOM	2495	CA	LEU	350	39.971	-7.610	64.352	1.00 32.43	В.
										•
	MOTA	2496	CB	LEU	350	41.112	-8.602	64.087	1.00 32.67	В
05	MOTA	2497	CG	LEU	350	41.782	-8.523	62.709	1.00 33.86	· B
25	MOTA	2498	CD1	LEU	350	41.867	-7.089	62.243	1.00 35.72	В
	ATOM	2499	CD2	LEU	350	43.160	-9.140	62.777		В
	MOTA	2500	C	LEU	350	38.880	-8.268	65.203	1.00 32.13	В
	MOTA	2501	0	LEU	350	37.869	-8.736	64.693	1.00 31.89	В
20	MOTA	2502	N	GLU	351	39.104	-8.286	66.510	1.00 32.99	· в
30	MOTA	2503	CA	GLU	351	38.163	-8.869	67.452	1.00 33.24	В
	MOTA	2504	СВ	GLU	351	38.807	-8.951	68.837	1.00 36.70	В
	ATOM	2505	CG	GLU	351	38.014	-9.772	69.821	1.00 44.06	В
•										
	ATOM	2506	CD	GLU	351		-11.179	69.309	1.00 47.54	В
25	ATOM	2507		GLU	351	38.805	-11.848	68.982	1.00 48.67	В
35	ATOM	· 2508	OE3	GLU	351	36.610	-11.599	69.228	1.00 48.07	В
	MOTA	2509	С	GLU	351	36.901	-8.009	67.519	1.00 31.83	В
	MOTA	2510	0	GLU	351	35.778	-8.532	67.584	1.00 32.55	В
	ATOM	2511	N	TYR	352	37.097				
							-6.690	67.503		В
40	MOTA	2512	CA	TYR	352	35.997	-5.727	67.550	1.00 25.10	В
40	MOTA	2513	CB	TYR	352	36.561	-4.318	67.758	1.00 23.54	В
	MOTA	2514	CG	TYR	352	35.537	-3.220	67.970	1.00 23.52	В
	.ATOM	2515	CD1	TYR	352	34.862	-2.642	66.893	1.00 21.07	В
	ATOM	2516		TYR	352	33.952	-1.601	67.086		
									1.00 22.50	В
15	MOTA	2517		TYR	352	35.271	-2.734	69.254	1.00 23.10	В
45	MOTA	2518	CE2	TYR	352	34.366	-1.699	69.464	1.00 22.61	В
	ATOM	2519	CZ	TYR	352	33.712	-1.134	68.377	1.00 25.05	В
	ATOM	2520	ОН	TYR	352	32.840	-0.085	68.577	1.00 29.15	В
	ATOM	2521	С	TYR	. 352	35.169	-5.790	66.262	1.00 23.04	В
50	ATOM	2522	0	TYR	352	33.957	-5.819	66.309	1.00 21.96	В
JU	MOTA	2523	N	ALA	353	35.841	-5.821	65.117	1.00 21.97	В
	MOTA	2524	CA	ALA	353	35.155	-5.883	63.826	1.00 24.73	В
	ATOM	2525	CB	ALA	353	36.163	-5.732	62.692	1.00 21.20	. В
	ATOM	2526	С	ALA	353	34.380	-7.192	63.663	1.00 26.52	В
	ATOM	2527	ŏ	ALA	353	33.283	-7.210	63.119		
55									1.00 25.94	В
JJ	ATOM	2528	N	HIS	354	34.978	-8.282	64.138	1.00 30.11	В
	MOTA	2529	CA	HIS	354	34.375	-9.607	64.052	1.00 32.42	В
	ATOM	2530	CB	HIS	354	35.334	-10.660	64.626	1.00 35.26	В
	MOTA	2531	CG	HIS	354		-12.073	64.317	1.00 38.11	В
	ATOM	2532		HIS	354		-13.045	65.103	1.00 38.24	
60 ·										В
oo	ATOM	2533	ND1		354		-12.614	63.053	1.00 39.29	В
	ATOM	2534		HIS	354		-13.858	63.072	1.00 38.94	В
	MOTA	2535	NE2	HIS	354	34.213	-14.143	64.303	1.00 39.79	В
	ATOM	2536	С	HIS	354	33.050	-9.642	64.811	1.00 33.09	В
	ATOM	2537	ō	HIS	354		-10.127	64.297	1.00 33.51	
65										В
5 5	MOTA	2538	N	ARG	355	33.053	-9.122	66.034	1.00 33.22	В
	MOTA	2539	CA	ARG	355	31.847	-9.091	66.852	1.00 35.31	В
	ATOM	2540	CB	ARG	355	32.145	-8.470	68.220	1.00 38.27	В
	MOTA	2541	CG	ARG	355	32.976	-9.320	69.155	1.00 41.93	В
	ATOM	2542	CD	ARG	355	33.322	-8.539	70.416	1.00 44.68	В
70	ATOM	2543	NE	ARG	355	32.132				
							-8.099	71.142	1.00 46.84	В
	MOTA	2544	CZ	ARG	355	31.299	-8.915	71.781	1.00 48.76	В
	MOTA	2545	NH1		355	31.523	-10.222	71.785	1.00 48.40	В
	MOTA	2546	NH2	ARG	355	30.243	-8.423	72.420	1.00 47.82	В

	MOTA	2547	С	ARG	355	30.7	40	-8.281	66.173	1.00 3	5.52	В
	MOTA	2548	ō	ARG	355	29.5		-8.610	66.297	1.00 3		В
	ATOM	2549	N	ALA	356	. 31.1		-7.228	65.454	1.00 3	3.02	В
_	MOTA	2550	CA	ALA	356	30.1	46	-6.374	64.789	1.00 3	1.19	В
5	MOTA	2551	CB	ALA	356	30.8		-5.156	64.206	1.00 3		В
	ATOM	2552	С	ALA	356	29.3		-7.089	63.704	1.00 3		В
	MOTA	2553	0	ALA	356	28.2		-6.645	63.343	1.00 2		В
	ATOM	2554	N	LYS	357	29.8		-8.197	63.194	1.00 3		В
10	MOTA MOTA	2555 2556	CA CB	LYS LYS	357 357	29.2		-8.973 -10.198	62.144 61.768	1.00 3		B B
10	ATOM	2557	CG	LYS	357			-9.906	61.350	1.00 3		· B
	ATOM	2558	CD	LYS	357			-10.458	59.956	1.00 3		В
	ATOM	2559	CE	LYS	357			-11.968	59.851	1.00 4		В
	ATOM	2560	NZ	LYS	357	32.4		-12.795	60.666	1.00 4		В
15	MOTA	2561	C	LYS	357	27.8		-9.447	62.552	1.00 3		В
	MOTA	2562	0	LYS	357	26.9	11	-9.512	61.724	1.00 3		В
	MOTA	2563	. N	ASN	358	27.6	54	-9.773	63.833	1.00 3	4.87	B
	MOTA	2564	CA	asn	358	26.3		-10.253	64.379	1.00 3		В
20	ATOM	2565	CB	ASN	358	26.6		-10.942	65.724	1.00 3		В
20	ATOM	2566	CG	ASN	358	27.5		-12.159	65.606	1.00 3		B
	ATOM	2567		ASN	358			-12.602	66.589	1.00 4		В
	ATOM .	2568		ASN	358	27.5		-12.713	64.404	1.00 3		В
	MOTA MOTA	2569 2570	C O	ASN ASN	358 358	25.3 24.4		-9.170 -9.322	64.574 65.406	1.00 3 1.00 3		B B
25	ATOM	2571	N	ILE	359	25.4		-8.076	63.825	1.00 3		· B
	ATOM	2572	CA	ILE	359	24.4		-7.003	63.951	1.00 4		В
	ATOM	2573		ILE	359	25.0		-5.608	63.869	1.00 4		В
	ATOM	2574		ILE	359	24.0		-4.529	63.858	1.00 4		В
	ATOM	2575	CG1	ILE	359	26.0	19	-5.402	65.066	1.00 4	0.61	В
30	MOTA	2576	CD1	ILE	359	26.8		-4.161	64.970	1.00 3		В
	ATOM	2577	С	ILE	359	23.3		-7.132	62.847	1.00 4		В
	ATOM	2578	0	ILE	359	23.7		-7.227	61.671	1.00 4		В
	ATOM	2579	N	LEU	360.	22.1		-7.140	63.241	1.00 4		B
35	ATOM	2580	CA CB	LEU	360	21.0		-7.276	62.293	1.00 4		В
55	MOTA MOTA	2581 2582	CG	LEU	360 360	19.9 19.6		-8.212 -9.524	62.864 62.123	1.00 5		B ·
	ATOM	2583		LEU	360	18.8		-10.456	63.043	1.00 5		В
	MOTA	2584		LEU	360	18.8		-9.248	60.836	1.00 5		В
	MOTA	2585	c	LEU	360	20.4		-5.927	61.966	1.00 4		В
40	ATOM	2586	ō	LEU	360	19.9		-5.211	62.854	1.00 4		B
	ATOM	2587	N	ASN	361	20.3	80	-5.586	60.681	1.00 4	7.32	В
	MOTA	2588	CA	ASN	361	19.8	05	-4.320	60.242	1.00 4	8.31	В
	MOTA	2589	CB	ASN	361	20.8		-3.502	59.458	1.00 4		В
45	MOTA	2590	CG	ASN	361	21.7		-2.743	60.360	1.00 4		·B
45	ATOM	2591		ASN	361	22.4		-1.777	59.933	1.00 4		В
	MOTA	2592		ASN	. 361	21.9		-3.175	61.609	1.00 4		В
	MOTA	2593	C	ASN	361	18.5		-4.526	59.387	1.00 4		В
	MOTA MOTA	2594 2595	И	ASN LYS	361 362	18.2 17.8		-5.627 -3.443	58.919 59.180	1.00 5 1.00 5		B B
50	MOTA	2596	CA	LYS	362	16.5		-3.452	58.400	1.00 5		В
	MOTA	2597	CB	LYS	362	16.8		-3.545	56.896	1.00 5		В
	MOTA	2598	CG	LYS	362	17.2		-2.229	56.253	1.00 4		В
	ATOM	2599	CD	LYS	362	17.1		-2.268	54.740	1.00 4		В
	MOTA	2600	CE	LYS	362	15.6	43	-2.244	54.329	1.00 4	7.35	В
55	MOTA	2601	NZ	LYS	362	14.9		~0.914	54.515	1.00 4		В
	MOTA	2602	С		362	15.6		-4.588	58.814	1.00 5		В
	ATOM	2603	0	LYS	362	15.2		-5.329	57.913	1.00 5		В
	MOTA	2604		LYS	362	15.3		-4.712	60.031	1.00 5		В
60	ATOM	2605	MG	MG	2602	43.6		10.621	59.419	1.00 2		300
OO	MOTA MOTA	2606 2607	PB	ADP ADP	2600 2600	44.2 44.6		7.165 7.765	60.136 61.419	1.00 2		ADP ADP
	ATOM	2608		ADP	2600	43.8		5.630	60.325	1.00 2		ADP
	ATOM	2609		ADP	2600	43.0		7.920	59.552	1.00 2		ADP
	MOTA	2610	PA	ADP	2600	45.6		7.818	57.697	1.00 3		ADP
65	ATOM	2611		ADP	2600	44.6		7.286	56.772	1.00 3		ADP
	MOTA	2612		ADP	2600	45.4		9.276	57.778	1.00 4		ADP
	MOTA	2613		ADP	2600	45.4		7.167	59.121	1.00 3		ADP
	ATOM	2614			2600	47.0		7.550	57.187	1.00 3		ADP
70	MOTA	2615		ADP	2600	48.1		6.858	57.828	1.00 4		ADP
70	MOTA	2616		ADP	2600	49.3		6.940	56.825	1.00 4		ADP
	MOTA	2617		ADP	2600	49.3		5.696	56.137	1.00 4		ADP
	MOTA	2618		ADP	2600	49.2		8.021	55.715	1.00 4		ADP
	MOTA	2619	03*	ADP	2600	50.5	12	8.717	55.502	1.00 4	9.03	ADP

	ATOM	2620	C2*	ADP	2600	48.810	7.296	54.462	1.00 46.75	ADP
	ATOM	2621	02*	ADP	2600	49.235	7.921	53.240	1.00 48.13	ADP
	MOTA	2622	C1 *	ADP	2600	49.328	5.886	54.701	1.00 47.35	ADP
_	ATOM	2623	N9	ADP	2600	48.435	4.815	54.144	1.00 48.03	ADP
5	ATOM	2624	C8	ADP	2600	47.417	4.221	54.811	1.00 47.72	ADP
_										
	ATOM	2625	N7	ADP	2600	46.839	3.328	54.046	1.00 48.56	ADP
	ATOM '	2626	C5	ADP	2600	47.454	3.316	52.892	1.00 49.10	ADP
	ATOM	2627	C6	ADP	2600	47.308	2.603	51.707	1.00 49.07	ADP
	MOTA	2628	N6	ADP	2600	46.350	1.680	51.610	1.00 49.43	ADP
10	ATOM	2629	Nl	ADP	2600	48.159	2.844	50.628	1.00 50.04	ADP
	ATOM	2630	C2	ADP	2600	49.152	3.776	50.684	1.00 48.98	
										ADP
	ATOM	2631	N3	ADP	2600	49.301	4.478	51.842	1.00 50.49	ADP
	ATOM	2632	C4	ADP	2600	48.491	4.283	52.944	1.00 48.96	ADP
	ATOM	2633	C1	2-7	1	37.376	16.487	53.441	1.00 31.12	2-7
15										
IJ	MOTA	2634	C2	2-7	1	38.554	16.442	52.639	1.00 31.01	2-7
	MOTA	2635	C3	2-7	1	38.554	15.433	51.622	1.00 31.01	2-7
	ATOM	2636	C4	2-7	1	37.388	14.559	51.530	1.00 29.91	2-7
				2-7						
	MOTA	2637	C5		1	36.248	14.570	52.396	1.00 29.25	2-7
	ATOM	2638	C6	2-7	1	36.296	15.546	53.415	1.00 30.61	2-7
20	ATOM	2639	C10	2-7	1	39.708	15.357	50.686	1.00 30.99	2-7
	MOTA	2640		2-7	1	40.272		50.056	1.00 33.35	2-7
							16.598			
	ATOM	2641	N12	2-7	1	41.446	16.158	49.317	1.00 33.73	2-7
	ATOM	2642	C13	2-7	1	41.189	14.730	49.013	1.00 31.60	2-7
	ATOM	2643		2-7	1	40.419	14.175	50.202	1.00 30.03	2-7
25										
23	MOTA	2644		2-7	1	41.032	14.136	47.645	1.00 28.72	2-7
	MOTA	2645	C19	2-7	1	42.014	13.131	47.164	1.00 27.73	2-7
	MOTA	2646		2-7	1	41.952	12.752	45.765	1.00 26.29	2-7
	MOTA	2647		2-7	1	40.984	13.380	44.878	1.00 26.40	2-7
	MOTA	2648	C22	2-7	1	39.931	14.256	45.351	1.00 27.79	2-7
30	ATOM	2649	C23	2-7	1	39.958	14.694	46.762	1.00 27.64	2-7
				2-7	ī.					
	ATOM	2650				42.438	17.110	49.102	1.00 34.81	2-7
	MOTA	2651	N30	2-7	1	43.717	16.767	49.283	1.00 35.06	2-7
	ATOM	2652	C31	2-7	1	44.603	17.929	49.086	1.00 31.67	2-7
	ATOM	2653		2-7	1	44.177	15.446	49.734	1.00 32.58	2-7
35										
22	MOTA	-2654		2-7	1	42.187	18.279	48.762	1.00 35.09	2-7
	MOTA	2655	F40	2-7	1	37.369	13.692	50.535	1.00 32.42	2-7
	ATOM	2656	E41	2-7	1	37.291	17.497	54.277	1.00 33.09	2-7
	MOTA	2657	0	нон	2		. 10.603	62.535	1.00 3.96	S
	ATOM	2658	0	нон	3	28.064	20.853	56.798	1.00 15.26	S
40	MOTA	2659	0	HOH	4	43.423	-1.052	63.682	1.00 6.84	s
	MOTA	2660	0	нон	5	41.471	9.650		1.00 28.56	S
	ATOM	2661	0	HOH	6	53.043	-17.874	61.146	1.00 22.21	S
	ATOM	2662	0	HOH	8	43.351	23.546	43.947	1.00 14.88	S
45	MOTA	2663	0	нон	11	31.538	6.420	79.791	1.00 20.07	s
43	ATOM	2664	0	нон	12	44.364	1.570	53.833	1.00 33.76	s
	ATOM	2665	0	HOH	13	42.141	-0.803	71.483	1.00 23.37	S
	ATOM	2666	Ō	нон	17	50.048	-0.508	68.644	1.00 38.33	Š
	MOTA	2667	0	нон	18	42.525	8.183	64.075	1.00 31.71	S
	ATOM	2668	0	нон	20	49.961	-5.304	63.635	1.00 28.76	S
50	MOTA	2669	0	HOH	21	52.974	11.228	41.771	1.00 27.37	s
-										
	MOTA	2670	0	нон	23	44.880	17.208	64.490	1.00 19.87	S
	MOTA	2671	0	нон	25	33.865	11.390	57.228	1.00 14.50	S
	MOTA	2672	0	HOH	26	42.746	19.345	56.865	1.00 19.80	S
	ATOM	2673	Ó	нон	27	43.217	3.216	42.636	1.00 29.84	Š
55										
22	MOTA	2674	0	нон	28	47.542	18.783	69.096	1.00 24.56	S
	ATOM	2675	0	нон	29	29.606	-8.997	58.639	1.00 41.51	S
	MOTA	2676	0	нон	30	38.143	15.249	61.346	1.00 12.36	s
	MOTA	2677	0	нон	31	47.769	14.311	41.568	1.00 24.48	s
	ATOM	2678	0	нон	32	22.227	19.477	42.995	1.00 35.68	S
60 -	MOTA	2679	0	нон	34	38:077	4.715	80.434	1.00 19.14	s
										5
	MOTA	2680	0	нон	35	27.208	25.794	60.457	1.00 30.49	S
	MOTA	2681	0	нон	40	45.874	21.711	68.966	1.00 14.93	S
	MOTA	2682	0	нон	42	37.931	3.241	64.945	1.00 21.80	S
	MOTA	2683								
65			0	нон	44	33.173	12.293	71.900	1.00 38.67	s
UJ	MOTA	2684	0	нон	45	38.986	3.636	49.470	1.00 20.20	S
	MOTA	2685	0	HOH	46	35.162	19.890	41.213	1.00 25.42	S
	MOTA	2686	ŏ	нон	52	22.755	-3.615			
								56.949	1.00 33.63	S
	MOTA	2687	0	HOH	53	27.917	6.206	79.432	1.00 19.49	S
	MOTA	2688	0	нон	55	37.862	4.182	47.024	1.00 13.89	S
70	MOTA	2689	ō	нон	57	31.462	4.272	82.519	1.00 37.59	Š
										3
	MOTA	2690	0	нон	59	38.826	12.586	58.140	1.00 18.34	s
	ATOM	2691	Ο.	HOH	60	27.879	4.380	76.644	1.00 24.90	S
	MOTA	2692	ō.	нон	61	45.041	10.037	53.740	1.00 42.66	š
			-			-2.017	,	22.740	42.00	J

	MOTA	2693	0	нон	62	28.763 26.533 62.454 1.00 35.09 S
	ATOM	2694	0	нон	66	38.448 -0.512 37.739 1.00 44.71 s
	MOTA	2695	0	нон	67	31.394 24.733 63.775 1.00 40.50 S
~	MOTA	2696	0	нон	68	40.487 5.787 72.041 1.00 37.21 S
5	MOTA	2697	0	HOH	69	52.548 19.976 38.009 1.00 24.27 S
	ATOM .	2698	Ο.	HOH	70	40.043 -1.641 68.804 1.00 21.10 ; S
	MOTA	2699	0	HOH	71	21.370 18.117 39.097 1.00 47.89 S
	MOTA	2700	0	нон	73	45.431 -1.388 51.309 1.00 36.21 S
	ATOM	2701	0	нон	74	12.109 0.216 54.870 1.00 45.32 S
10	MOTA	2702	0	нон	78	41.390 5.467 40.236 1.00 31.36 S
	ATOM	2703	ō	нон	79	38.398 -10.202 49.709 1.00 28.25 S
	ATOM	2704	ō	нон	84	46.457 -1.971 63.989 1.00 20.69 S
	ATOM	2705	ō	нон	87	2.291 6.433 36.064 1.00 27.27 S
	MOTA	2706	ŏ	нон	88	46.187 3.359 74.292 1.00 30.60 S
15	ATOM	2707	ŏ	нон	89	51.911 4.577 56.634 1.00 44.94 S
	ATOM	2708	ŏ	нон	90	45.811 18.580 66.703 1.00 26.87 S
	ATOM	2709	ŏ	нон	91	47.734 13.013 72.702 1.00 32.94 S
	ATOM	2710	ŏ	нон	92	23.555 15.386 53.064 1.00 29.56 S
	ATOM	2711	ŏ	нон	93	43.670 -2.643 73.172 1.00 27.18 S
20	ATOM	2711	ŏ	НОН	94	27.978 20.947 70.487 1.00 41.48 S
20	ATOM	2713	ŏ	нон	95	44.678 -7.048 71.862 1.00 24.48 S
	ATOM	2714	Ö	нон	97	37.124 2.776 73.009 1.00 36.39 S
	ATOM	2715	0	HOH	98	
			-			
25	ATOM	2716	0	нон	101	46.793 22.739 62.116 1.00 28.62 s
23	ATOM	2717	0	нон	104	20.079 21.304 46.635 1.00 44.83 S
	ATOM	2718	0	нон	105	30.653 -3.670 75.744 1.00 35.11 s
	ATOM	2719	0	нон	106	46.987 13.182 34.815 1.00 16.99 S
	MOTA	2720	0	нон	109	43.794 0.066 55.803 1.00 30.02 s
30	ATOM	2721	0	нон	111	25.208 9.102 28.662 1.00 32.86 S
30	ATOM	2722	0	нон	113	44.655 15.401 59.741 1.00 25.68 s
	MOTA	2723	0	HOH	115	18.285 12.456 33.587 1.00 30.40 S
	MOTA	2724	0	нон	116	47.999 -0.217 48.915 1.00 36.92 S
	MOTA	2725	0	HOH	117	23.508 25.313 66.864 1.00 47.95 S
25	MOTA	2726	0	HOH	119	27.220 -14.904 55.904 1.00 35.41 S
35	ATOM	2727	0	нон	120	47.343 8.255 68.520 1.00 37.89 S
	ATOM	2728	0	нон	128	28.608 -6.298 48.882 1.00 26.00 S
	ATOM	2729	0	нон	132	6.107 15.208 42.672 1.00 30.09 S
	ATOM	2730	0	HOH	133	26.812 14.766 57.900 1.00 17.88 S
in	ATOM	2731	0	HOH	135	46.950 10.746 67.779 1.00 31.59 S 24.332 1.606 79.565 1.00 28.86 S
40	ATOM	2732	0	нон	136	24.332 1.606 79.565 1.00 28.86 S
	ATOM	2733	0	нон	138	50.215 2.473 62.680 1.00 35.95 S
	ATOM	2734	0	нон	139	22.069 24.748 54.683 1.00 25.56 S
	MOTA	2735	0	нон	140	44.497 -18.491 58.486 1.00 49.65 S
	ATOM	2736	ò	нон	141	15.900 -4.594 62.687 1.00 33.93 S
45	ATOM	2737	ō	нон	143	14.793 -3.866 47.507 1.00 45.81 S
	END		-			

TABLE 4

	D COVE DV		3.54Y					L =	•		
						1-2a_2dp					
5 .	! CRYST		.200		.400			.00 90.0		P212121	
J .	ATOM ATOM	2605	CB	LYS	17			-12.132	60.197	1.00 50.9	_
•	ATOM	2606	CG	LYS	17			-12.714	59.720	1.00 53.4	
		2607 2608	CD	LYS	17			-12.276	58.298	1.00 55.1	
	ATOM ATOM		CE	LYS	17			-13.129	57.240 57.341	1.00 56.4	
10	ATOM	2609 2610	. NZ C	LYS LYS	17 17		464	-13.074		1.00 55.9	
10	ATOM	2611	Ö	LYS	17		371	-9.793 -9.870	59.322	1.00 46.3	
•	MOTA	2612	N	LYS	17			-10.326	58.525		
	ATOM	2613	CA	LYS	17			-10.520	61.434 60.578	1.00 49.0	
•	MOTA	2614	N	ASN	18		441	-8.969	59.167	1:00 44.0	
15	MOTA	2615	CA	ASN	18		346	-8.128	57.990	1.00 44.0	
10	ATOM	2616	CB	ASN	18		016	-7.375	58.014	1.00 42.8	
	ATOM	2617	CG	ASN	18		059	-7.856	56.934	1.00 45.6	
	ATOM	2618		ASN	18		222		55.748	1.00 47.6	
	ATOM	2619		ASN	18		068	-8.642	57.331	1.00 46.0	
20	ATOM	2620	C	ASN	18		508	-7.150		1.00 40.2	
	ATOM	2621	ō	ASN	18		895	-6.921	56.596	1.00 42.1	
	ATOM	2622	N	ILE	19		077	-6.584	58.810	1.00 36.3	
	ATOM	2623	CA	ILE	19		171	-5.618	58.668	1.00 32.3	
	ATOM	2624	CB	ILE	19		495	-4.982	60.043	1.00 33.0	
25	ATOM	2625	CG2	ILE	19		959	-6.042	61.012	1.00 34.8	
	MOTA	2626	CG1	ILE	19		599	-3.938	59.905	1.00 33.8	
	ATOM	2627	CD1	ILE	19	27.	845	-3.169	61.165	1.00 32.2	
	ATOM	2628	C	ILE	19	27.	464	-6.184	58.058	1.00 28.4	
	ATOM	2629	0	ILE	19	28.	021	-7.161	58.574	1.00 29.0	
30	ATOM .	2630	N	GLN	20	27.	934	-5.566	56.967	1.00 22.2	
•	MOTA	2631	CA	GLN	20	29.	174	-5.986	56.285	1.00 15.9	
	MOTA	2632	CB	GLN	20	29.	216	-5.493	54.839	1.00 14.8	2 B
•	MOTA .	2633	CG	GLN	20	30.	526	-5.834	54.127	1.00 14.6	8 B
25	MOTA	2634	CD	GLN	20	30.	589	-5.290	52.715	1.00 13.6	0 в
35	MOTA	2635		GLN	20	30.	540	-4.089	52.514	1.00 13.4	7 B
	ATOM	2636		GLN	20		720	-6.173	51.737	1.00 13.0	4 B
	MOTA	2637	C	GLN	20		450	-5.437	56.952	1.00 13.2	5 B
	MOTA	2638	0	GLN	20		566	-4.239	57.180	1.00 12.3	3 в
40	ATOM	2639	N	VAL .			394	-6.328	57.254	1.00 9.3	
40	ATOM	2640	CA	VAL	21		656	-5.941	57.880	1.00 6.2	
	ATOM	2641	CB	VAL	21		775	-6.537	59.296	1.00 5.9	
	ATOM	2642		VAL	21		094	-6.144	59.934	1.00 3.4	
	ATOM	2643		VAL	21		616	-6.056	60.138	1.00 7.7	
45	MOTA	2644	C	VAL	21		868	-6.396	57.052	1.00 5.0	
73	MOTA	2645	0.	VAL	21		031	-7.569		1.00 4.2	
	ATOM ATOM	2646 2647	N CA	VAL VAL	22 22		715	-5.454	56.659	1.00 3.7	
	MOTA	2648	CB	VAL	22		893 819	-5.805 -5.226	55.879 54.420	1.00 4.1	
	ATOM	2649		VAL	22		566	-5.731	53.703	1.00 3.3 1.00 3.1	
50	ATOM	2650		VAL	22		823	-3.717	54.452	1.00 3.1 1.00 2.8	
	ATOM	2651	C	VAL	22		157	-5.305	56.553	1.00 6.2	
	ATOM	2652	ō	VAL	22		122	-4.365	57.352	1.00 6.7	
	ATOM	2653	N	VAL	23		271	-5.946	56.223	1.00 4.4	
	ATOM	2654	CA	VAL	23		559	-5.585	56.785	1.00 4.2	
55	ATOM	2655	CB	VAL	23		195	-6.830	57.477	1.00 4.0	
	ATOM	2656	CG1	VAL	23		555	-6.511	58.081	1.00 1.8	
	MOTA	2657	CG2		23		268	-7.319	58.550	1.00 5.7	
		2658	C	VAL	23		505	-5.037	55.710	1.00 4.4	
		2659	0	VAL	23		553	-5.531	54.586	1.00 4.6	
60		2660	N	ARG	24		251	-3.998	56.057	1.00 7.2	
		2661	CA	ARG	24		228	-3.436	55.128	1.00 9.8	
		2662	СВ	ARG	24		793	-2.092	54.531	1.00 6.5	
		2663	CG	ARG	24		744	-1.662	53.425	1.00 6.8	
		2664	CD	ARG	24		401	-0.306	52.837	1.00 7.9	
65		2665	NE	ARG	24		142	-0.040	51.603	1.00 4.8	
		2666	CZ	ARG	24		041	1.095	50.909	1.00 3.4	
		2667	NH1		24		228	2.056	51.329	1.00 1.0	
		2668	NH2		24		773	1.287	49.814	1.00 1.0	
		2669	С	ARG	24	43.		-3.179	55.856	1.00 13.0	
70		2670	0	ARG	24		586	-2.374	56.791	1.00 13.4	
	MOTA	2671	N _.	CYS	25	44.		-3.873	55.421	1.00 13.8	

	ATOM	2672	CA	CYS	25	45.928	-3.742	55.996	1.00 16.78	В
	MOTA	2673	СВ	CYS	25	46.646	-5.088	55.932	1.00 14.53	В
	MOTA	2674	SG	CYS	25	48.149	-5.147	56.865	1.00 15.92	
				CYS					1.00 15.92	В
5	MOTA	2675	Č		25	46.743	-2.706	55.216		В
,	MOTA	2676	0	CYS	25	46.793	-2.743	53.991	1.00 19.83	В
	ATOM .	2677	N	ARG	26	47.369	-1.774	55.922	1.00 20.13	В
	MOTA	2678	CA	ARG	26	48.186	-0.779	55.242	1.00 23.56	В
	ATOM	2679	CB	ARG	26	48.410	0.441	56.122	1.00 23.04	В
• •	MOTA	2680	CG	ARG	26	49.018	0.108	57.480	1.00 25.34	В
10	MOTA	2681	CD	ARG	26	49.478	1.335	58.248	1.00 25.85	В
	ATOM	2682	NE	ARG	26	50.882	1.635	57.970	1.00 27.66	· В
	MOTA	2683	CZ	ARG	26	51.876	1.425	58.830	1.00 29.35	В
	MOTA	2684		ARG	26	51.620	0.914	60.030	1.00 28.00	В
	MOTA	2685		ARG	26	53.126	1.729	58.494	1.00 29.65	В
15	ATOM	2686	C	ARG	26	49.566	-1.360	54.924	1.00 26.17	В
10	ATOM	2687	ō	ARG	26	49.965	-2.367	55.500	1.00 27.47	
										. В
	MOTA	2688	N_	PRO	27	50.296	-0.748	53.976	1.00 28.46	В
	MOTA	2689	CD	PRO	27	49.815	0.221	52.972	1.00 28.96	В
20	MOTA	2690	CA	PRO	27	51.634	-1.225	53.617	1.00 30.05	В
20	MOTA	2691	CB	PRO	27	51.757	-0.791	52.157	1.00 29.21	В
	MOTA	2692	CG	PRO	27	51.081	0.508	52.153	1.00 27.78	В
	ATOM .	2693	С	PRO	27	52.652	-0.565	54.551	1.00 30.74	В
	ATOM	2694	0	PRO	27	52.315	0.387	55.255	1.00 30.33	В
	MOTA	2695	N	PHE	28	53.888	-1.065	54.559	1.00 33.00	В
25	ATOM	2696	CA	PHE	28	54.946	-0.488	55.397	1.00 35.47	В
	ATOM	2697	CB	PHE	28	56.197	-1.349	55.423		. В
	ATOM	2698		PHE	28	56.043	-2.621	56.180	1.00 34.30	В
	MOTA	2699			28					
				PHE		55.970	-3.848	55.506	1.00 33.11	В
30	MOTA	2700		PHE	28	55.975	-2.598	57.566	1.00 34.50	В
JU	MOTA	2701		PHE	28	55.831	-5.030	56.204	1.00 32.04	В
	MOTA	2702	-	PHE	28	55.833	-3.779	58.283	1.00 34.83	В
	MOTA	2703	CZ	PHE	28	55.762	-5.002	57.594	1.00 34.76	В
	MOTA	2704	С	PHE	28	55.432	0.848	54.837	1.00 37.44	В
	ATOM	2705	0	PHE	28	55.529	1.019	53.640	1.00 37.96	В
35	ATOM	2706	N	ASN	29	55.724	1.797	55.719	1.00 41.21	В.
	MOTA	2707	CA	ASN	29	56.195	3.114	55.288	1.00 43.97	В
	ATOM	2708	СB	ASN	29	55.731	4.190	56.280	1.00 42.30	В
	ATOM	2709	CG	ASN	29	56.080	3.843	57.724	1.00 41.84	В
	ATOM	2710		ASN	29	57.230	3.554	58.038	1.00 40.87	В
40	MOTA	2711		ASN	29	55.080		58.604		
							3.866		1.00 40.16	В
	MOTA	2712	C	ASN	29	57.718	3.112	55.190	1.00 47.03	В
	ATOM	2713	0	ASN	29	58.361	2.179	55.651	1.00 48.57	В
	ATOM	2714	N	LEU	30	58.290	4.156	54.594	1.00 49.85	В
45	MOTA	2715	CA	LEU	30	59.745	4.258	54.442	1.00 52.56	В
43	MOTA	2716	CB	LEU	30	60.125	5.641	53.928	1.00 52.63	В
	MOTA	2717	CG	LEU	. 30	60.214	5.735	52.409	1.00 53.20	В
	MOTA	2718	CD1	LEU	30	60.395	7.194	51.973	1.00 53.18	В
	MOTA	2719	CD2	LEU	30	61.378	4.862	51.935	1.00 54.30	В
	ATOM	2720	С	LEU	30	60.579	3.978	55.695	1.00 54.36	В
50	ATOM	2721	0	LEU	30	61.623	3.347	55.619	1.00 54:97	В
	ATOM	2722	N	ALA	31	60.121	4.453	56.847	1.00 56.36	В
	ATOM	2723	CA	ALA	31	60.843	4.228	58.097	1.00 58.76	В
	ATOM	2724	CB	ALA	31	60.214	5.057	59.202	1.00 58.55	В
	ATOM	2725	Ċ	ALA	31	60.842	2.742	58.487	1.00 60.40	В
55	ATOM	2726	ŏ	ALA	31	61.749	2.266	59.167	1.00 60.67	В
-	ATOM	2727	N	GLU		59.819	2.016	58.045		
									1.00 61.95	В
	MOTA	2728	CA	GLU	32	59.692	0.594	58.350	1.00 63.39	В
	ATOM	2729	CB	GLU	32	58.215	0.187	58.322	1.00 62.91	В
6 0	ATOM	2730	CG	GLU	32	57.429	0.683	59.524	1.00 62.16	В
60	ATOM	2731	CD	GLU	32	55.933	0.669	59.299	1.00 61.37	В
	MOTA	2732		GLU	32	55.191	0.841	60.289	1.00 60.97	В
	MOTA	2733	OE2	GLU	32	55.504	0.497	58.138	1.00 60.36	В
	ATOM	2734	С	GLU	32	60.487	-0.318	57.414	1.00 64.76	В
	MOTA	2735	0	GLU	32	61.130	-1.261	57.860	1.00 64.21	В
65	MOTA	2736	N	ARG	33	60.436	-0.039	56.116	1.00 66.90	В
-	ATOM	2737	CA	ARG	33	61.150	-0.855	55.141	1.00 69.19	B
	ATOM	2738	CB	ARG	33	60.690	-0.503	53.719	1.00 70.74	
	ATOM	2739	CG	ARG	33				1.00 70.74	В
	ATOM	2740				60.911	0.953	53.310		В
70		2741	CD	ARG	33	60.238	1.267	51.977	1.00 75.17	В
, 0	MOTA		NE	ARG	33	60.663	0.349	50.920	1.00 76.52	В
	MOTA	2742	CZ	ARG	33	61.889	0.301	50.400	1.00 76.92	В
	MOTA	2743		ARG	33	62.838	1.122	50.829	1.00 76.57	В
	MOTA	2744	NH2	ARG	33	62.168	-0.569	49.441	1.00 78.04	В

	MOTA	2745	С	ARG	33	62.650	-0.654	55.297	1.00 70.11	В
	ATOM	2746	0	ARG	33	63.439	-1.524	54.943	1.00 70.36	В
	MOTA	2747	N	LYS	34	63.038	0.500	55.832	1.00 71.13	В
_	MOTA	2748	CA	LYS	34	64.447	0.798	56.053	1.00 72.18	В
5	MOTA	2749	CB	LYS	34	64.623	2.254	56.498	1.00 73.21	В
	MOTA	2750	CG	LYS	34	64.611	3.267	55.363	1.00 74.27	В
	MOTA	2751	CD	LYS	34	66.023	3.637	54.921	1.00 74.99	В
	MOTA	2752	CE	LYS	34	66.769	2.463	54.306	1.00 74.88	В
	MOTA	2753	NZ	LYS	34	68.154	2.852	53.916	1.00 75.81	B
10	MOTA	2754	C	LYS	34	65.006	-0.137	57.123	1.00 72.12	В
10				LYS						
	MOTA	2755	. 0		34	66.207	-0.424	57.142	1.00 72.82	В
	MOTA	2756	N	ALA	35	64.130		58.007	1.00 71.37	В
	MOTA	2757	CA	ALA	35	64.522	-1.526	59.077	1.00 69.94	В
15	MOTA	2758	CB	ALA	35	63.780	-1.177	60.361	1.00 69.77	В
15	MOTA	2759	С	ALA	35	64.223	-2.970	58.685	1.00 69.24	В
	MOTA	2760	0	ALA	35	64.198	-3.854	59.542	1.00 69.32	B
	MOTA	2761	N	SER	36	64.001	-3.194	57.388	1.00 68.43	В
	MOTA	2762	CA	SER	36	63.689	-4.519	56.848	1.00 66.99	В
	MOTA	2763	CB	SER	36	64.937	-5.405	56.860	1.00 67.27	В
20	ATOM	2764	OG	SER	36	65.906	-4.912	55.959	1.00 67.40	В
	ATOM	2765	C	SER	36	62.579	-5.159	57.674	1.00 65.70	В
	ATOM	2766	ō	SER	36	62.721	-6.270	58.185	1.00 65.65	В.
	ATOM	2767	N	ALA	37	61.469	-4.435	57.791	1.00 64.41	В.
	ATOM	2768	CA	ALA	37	60.320	-4.880	58.568	1.00 62.00	·B
25	ATOM	2769	CB	ALA	37	59.256	-3.784	58.601	1.00 62.35	В
23										
	ATOM	2770	C	ALA	37	59.699	-6.185	58.093	1.00 59.79	В
	MOTA	2771	0	ALA	37	59.490	-6.404	56.909	1.00 58.90	В
	ATOM	2772	N	HIS	38 .	59.400	-7.042	59.061	1.00 58.16	В
30	MOTA	2773	CA	HIS	38	58.795	-8.347	58.828	1.00 55.57	В
30	MOTA	2774	CB	HIS	38	59.420	-9.381	59.785	1.00 57.59	В
	MOTA	2775	CG	HIS	38	59.426	-8.963	61.233	1.00 58.97	В
	MOTA	2776	CD2	HIS	38	58.878	-9.543	62.328	1.00 58.78	В
	MOTA	2777	ND1	HIS	38	60.083	-7.837	61.689	1.00 58.86	В
~-	MOTA	2778	CE1	HIS	38	59.939	-7.744	63.000	1.00 58.84	В
35	MOTA	. 2779	NE2	HIS	38	59.211	-8.766	63.412	1.00 58.91	В
	MOTA	2780	С	HIS	38	57.296	-8.223	59.086	1.00 53.05	В
	ATOM	2781	0	HIS	38	56.890	-7.787	60.163	1.00 54.10	В
	MOTA	2782	N	SER		56.472	-8.605	58.114	1.00 48.25	В
	ATOM	2783	CA	SER	39	55.026	-8.500	58.290	1.00 42.98	В
40	MOTA	2784	CB	SER	39	54.295	-8.575	56.970	1.00 42.55	В
	MOTA	2785	ŌĞ	SER	39	52.903	-8.490	57.201	1.00 39.13	В
	ATOM	2786	c	SER	39	54.444	-9.616	59.130	1.00 40.52	В
	ATOM	2787	ō	SER	39		-10.773	58.919	1.00 39.58	В
	MOTA				40					
45		2788	N	ILE		53.603	-9.247	60.092	1.00 38.79	В
73	ATOM	2789	CA	ILE	40		-10.222	60.979	1.00 36.32	В
	MOTA	2790	CB	ILE	40	53.039	-9.786	62.478	1.00 37.00	В
	ATOM	2791		ILE	40	54.493	-9.677	62.925	1.00 37.72	₿
	MOTA	2792		ILE	40	52.307	-8.458	62.692	1.00 37.68	В
50	ATOM	2793		ILE	40	52.102	-8.097	64.161	1.00 37.35	В
50	MOTA	2794	С	ILE	40	51.501	-10.426	60.611	1.00 34.00	В
	MOTA	2795	0	ILE	40	50.757	-11.084	61.319	1.00 32.93	В
	MOTA	2796	N	VAL	41	51.097	-9.863	59.482	1.00 33.39	В
	MOTA	2797	CA	VAL	41	49.720	-9.986	59.028	1.00 32.21	В
	ATOM	2798	СВ	VAL	41	48.982	-8.617	59.042	1.00 31.99	В
55	MOTA	2799	CG1	VAL	41	47.559	-8.778	58.536	1.00 30.52	В
	ATOM	2800		VAL	41	48.964	-8.048	60.445	1.00 32.73	В
	ATOM	2801	Č		41		-10.526		1.00 32.35	В
	АТОМ	2802	ŏ	VAL	41		-10.022	56.728	1.00 31.91	В
	MOTA	2803	N	GLU	42		-11.565	57.417	1.00 33.52	
60	MOTA	2804			42			56.112	1.00 34.79	В
00			CA	GLU			-12.189			В
	MOTA	2805	CB	GLU	42		-13.626	56.142	1.00 34.88	В
	MOTA	2806	CG	GLU	42		-13.762	55.882	1.00 35.91	В
	MOTA	2807	CD	GLU	42		-15.139	.56.222	1.00 36.62	В
65	MOTA	2808		GLU	42		-16.105	55.996	1.00 35.55	В
65	MOTA	2809		GLU	42		-15.262	56.704	1.00 36.67	В
	MOTA	2810	С	GLU	42		-12.207	55.689	1.00 34.67	В
	MOTA	2811	0	GLU	42	46.425	-12.745	56.388	1.00 35.11	В
	MOTA	2812	N	CYS	43	46.959	-11.615	54.540	1.00 33.53	В
	MOTA	2813	CA	CYS	43		-11.575	54.074	1.00 33.64	В
70	MOTA	2814	CB	CYS	43	45.241	-10.172	53.575	1.00 31.73	В
	ATOM	2815	SG	CYS	43	45.291	-8.913	54.863	1.00 30.24	В
	MOTA	2816	Ċ.	CYS	43		-12.597	52.985	1.00 34.68	В
	MOTA	2817	ō .	CYS	43		-12.722	52.025	1.00 35.47	В
							•			_

	MOTA	2818	N	ASP	44	44.220 -	13.335	53.160	1.00 34.51	В
	ATOM	2819	CA	ASP	44	43.821 -	14.347	52.196	1.00 35.72	В
	ATOM	2820	CB	ASP	44	43.698 -	15.710	52.875	1.00 37.74	В
	ATOM	2821	CG	ASP	44	43.627 -		51.880	1.00 39.14	В
5	ATOM	2822		ASP	44		16.681	50.787	1.00 38.15	B
-										
	MOTA	2823		ASP	44	44.166 -		52.206	1.00 40.23	В
	ATOM	2824	Ç	ASP	44	42.452 -		51.662	1.00 36.02	В
	ATOM	2825	0	ASP	44	41.433 -	14.323	52.228	1.00 34.41	В
	ATOM	2826	N	PRO	45	42.415 -	13.177	50.566	1.00 36.48	В
10	MOTA	2827	CD	PRO	45	43.558 -	12.792	49.725	1.00 37.08	В
	MOTA	2828	CA	PRO	45	41.162 -		49.962	1.00 36.44	• В
	MOTA	2829	CB	PRO	45	41.646 -		48.828	1.00 36.90	
										В
	MOTA	2830	CG	PRO	45	42.892 -		48.398	1.00 37.61	В
	MOTA	2831	С	PRO	45	40.254 -		49.518	1.00 36.95	В
15	MOTA	2832	0	PRO	45	39.046 -	13.805	49.685	1.00 37.27	В
	MOTA	2833	N	VAL	46	40.834 -	14.912	48.930	1.00 37.39	В
	MOTA		CA	VAL	46		16.057	48.479	1.00 37.62	В
	ATOM	2835	СВ	VAL	46		17.087	47.773	1.00 38.49	В
20	MOTA	2836		VAL	46		18.269	47.334	1.00 39.31	В
20	MOTA	2837		VAL	46	41.642 -		46.584	1.00 38.33	В
	ATOM	2838	С	VAL	46	39.354 -	16.728	49.665	1.00 37.65	В
	ATOM	2839	0	VAL	46	38.172 -:	17.082	49.606	1.00 38.03	В
	ATOM	2840	N	ARG	47	40.089 -	16.902	50.752	1.00 37.10	В
	ATOM	2841	CA	ARG	47	39.520 -		51.947	1.00 37.76	В
25	ATOM	2842	СВ	ARG	47	40.627 -		52.797	1.00 40.98	В
	ATOM	2843	CG	ARG	47	40.138 -		53.811	1.00 45.53	. В
	ATOM	2844	CD	ARG	47	40.088 -		53.205	1.00 48.08	В
	MOTA	2845	NE	ARG	47	41.427 -	21.065	52.905	1.00 51.05	В
	MOTA	2846	CZ	ARG	47	42.361 -	21.291	53.826	1.00 53.04	В
30	MOTA	2847	NH1	ARG	47	42.101 -		55.108	1.00 53.32	В
	ATOM	2848		ARG	47	43.558 -		53.467	1.00 53.55	В
	ATOM	2849	C	ARG	47	38.817 -		52.774	1.00 35.87	В
	ATOM	2850	0	ARG	47.	38.091 -		53.702	1.00 35.14	В
25	MOTA	2851	N	LYS	48	39.054 ~:		52.420	1.00 34.57	В
35	MOTA	2852	CA	LYS	48	38.456 -	14.051	53.125	1.00 32.91	В.
	MOTA	2853	CB	LYS	48	36.938 -:	14.158	53.092	1.00 34.16	В
	MOTA	2854	CG	LYS	48	36.361 -:	14.145	51.693	1.00 36.73	В
	MOTA	2855	CD	LYS	48	34.854 -		51.706	1.00 37.41	В
		2856								
40	MOTA		CE	LYS	48		14.550	50.314	1.00 38.70	B
40	MOTA	2857	NZ	LYS	48	34.704 -:		49.344	1.00 36.20	В
	ATOM	2858	С	LYS	48	38.903 -	13.978	54.578	1.00 31.33	В
	MOTA	2859	0	LYS	48	38.140 -	13.593	55.440	1.00 31.50	В
	ATOM	2860	N	GLU	49	40.151 -	14.352	54.836	1.00 29.95	В
	MOTA	2861	CA	GLU	49		14.330	56.193	1.00 27.26	B
45	ATOM	2862	CB	GLU	49		15.719	56.633	1.00 28.44	В
		2863								
	ATOM		CG	GLU	49		16.815	56.656	1.00 28.64	В
	MOTA	2864	CD	GLU	49	40.760 -		56.980	1.00 29.46	В
	MOTA	2865	OE1	GLU	49	40.028 -	19.168	56.992	1.00 29.37	В
	MOTA	2866	OE2	GLU	49	41.986 -:	18.211	57.220	1.00 29.95	В
50	ATOM	2867	С	GLU	49	41.924 -	13.438	56.344	1.00 24:62	В
	MOTA	2868	Ō	GLU	49		13.164	55.395	1.00 23.41	В
	MOTA	2869	N	VAL	50		12.973	57.565	1.00 23.85	В
	ATOM	2870	CA	VAL	50		12.164	57.915	1.00 22.58	
										В
55	MOTA	2871	CB	VAL	50		10.738	58.417	1.00 21.03	В
22	MOTA	2872		VAL	50		10.851	59.540	1.00 20.58	В
	MOTA	2873	CG2	VAL	50		-9.968	58.884	1.00 19.55	В
	MOTA	2874	С	VAL	50	43.909 -:	12.995	59.036	1.00 23.21	В
	MOTA	2875	0	VAL	50	43.234 -:		59.959	1.00 22.47	В
	ATOM	2876	N	SER	51	45.197 -		58.923	1.00 24.22	В
60	MOTA	2877								
00			CA	SER	51	45.867 -		59.950	1.00 26.05	В
	MOTA	2878	СВ	SER	51	46.398 -		59.352	1.00 26.43	В
	ATOM	2879	OG	SER	51	46.705 -:	16.299	60.383	1.00 26.88	В
	ATOM	2880	С	SER	51	47.013 -:	13.293	60.579	1.00 26.62	В
	MOTA	2881	0	SER	51	47.893 -		59.868	1.00 26.40	. в
65	ATOM	2882	N	VAL	52	46.998 -		61.908	1.00 27.16	В
	MOTA	2883	CA		52	48.000 -:				
				VAL				62.657	1.00 29.10	В
	MOTA	2884	CB	VAL	52	47.311 -:		63.640	1.00 28.02	В
	ATOM .	2885		VAL	52	48.336 -		64.340	1.00 27.20	В
- 0	MOTA	2886	CG2	VAL	52	46.341 -	10.607	62.885	1.00 27.34	В
70	MOTA	2887	С	VAL	52	48.974 -:	13.331	63.442	1.00 30.28	, В
	ATOM	2888	0	VAL	52	48.567 -		64.117	1.00 30.72	. В
	ATOM	2889	N	ARG	53	50.265 -		63.342	1.00 30.72	В
	MOTA	2890	CA							
	AT ON	2030	CA	ARG	53	51.276 -		64.070	1.00 32.95	В

	ATOM	2891	CB	ARG	53	52.615	-13:750	63.336	1.00 33.14	В
	ATOM	2892	CG	ARG	53	57 676	-14.706	63.926	1.00 32.63	В
	ATOM	2893	CD	ARG	53		-15.197	62.851	1.00 33.53	В
_	MOTA	2894	NE	ARG	53	55.482	-14.163	62.378	1.00 34.35	В
5	MOTA	2895	CZ	ARG	53	56.017	-14.140	61.161	1.00 35.36	В
	ATOM	2896	NH1		53		-15.089	60.272	1.00 35.11	В
	ATOM .			ARG			-13.162			B
		2897			53			60.838	1.00 36.70	
	MOTA	2898	С	ARG	53	51.423	-13.182	65.458	1.00 34.27	В
	MOTA	2899	0	ARG	53	51.964	-12.088	65.632	1.00 34.80	В
10	ATOM	2900	N	THR	54		-13.915	66.446	1.00 35.04	В
	MOTA	2901		THR	54		-13.458	67.815	1.00 37.72	В
			·CA							
	MOTA	2902	СВ	THR	54		-13.823	68.540	1.00 37.47	В
	ATOM	2903	0G1	THR	54 .	49.521	-15.244	68.581	1.00 36.02	В
	MOTA	2904	CG2	THR	54	48.484	-13.260	67.804	1.00 37.61	В
15	ATOM	2905	C	THR	54	-	-14.056	68.586	1.00 39.85	В
10						52.517				
	MOTA	2906	0	THR	54		-13.554	69.633	1.00 39.10	В
	MOTA	2907	N	GLY	55	52.721	-15.121	68.043	1.00 43.17	В
	ATOM	2908	CA	GLY	55	53.810	-15.791	68.727	1.00 48.23	В
	ATOM	2909	С	GLY	55	55.214	-15.667	68.165	1.00 51.61	. в
20	ATOM	2910	ō	GLY	55		~14.562	67.926	1.00 52.45	B
20										
	MOTA	2911	N	GLY	56	55.855	-16.820	67.962	1.00 53.22	В
	ATOM	2912	CA	GLY	56	57.219	-16.864	67.464	1.00 54.95	В,
	MOTA	2913	С	GLY	56	57.420	-16.365	66.052	1.00 56.66	В
	MOTA	2914	0	GLY	56		-15.450	65.611	1.00 57.44	• В
25	MOTA	2915			57		-16.980		1.00 57.72	В
25			N	LEU				65.346		
	MOTA	2916	CA	LEU	57		-16.600	63.972	1.00 58.30	В
	MOTA	2917	CB	LEU	57	60.219	-16.608	63.777	1.00 58.78	В
	MOTA	2918	CG	LEU	57 .	61:067	-17.384	64.790	1.00 59.20	В
	ATOM	2919		LEU	57		-18.870	64.762	1.00 59.75	· B
30										
50	MOTA	2920		LEU	57		-17.175	64.472	1.00 59.20	В
	ATOM	2921	С	LEU	57	58.029	-17.493	62.921	1.00 58.10	В
	ATOM	2922	0	LEU	57	57.153	-18.289	63.245	1.00 58.57	В
•	MOTA	2923	N	ALA	58		-17.343	61.665	1.00 57.02	В
	ATOM	2924	CA	ALA	58		-18.126	60.555	1.00 55.81	В
35 [°]										
22	MOTA	2925	CB	ALA	58		-17.615	59.235	1.00 55.75	В
	MOTA	2926	С	ALA	58	58.193	-19.622	60.705	1.00 54.88	В
	MOTA	2927	0	ALA	58	57.350	-20.460	60.375	1.00 54.40	В
	MOTA	2928	N	ASP	59	59 386	-19.937	61.211	1.00 53.60	В
40	MOTA	2929	CA	ASP	59		-21.316	61.431	1.00 51.49	В
40	MOTA	2930	CB	ASP	59		-21.290	62.050	1.00 51.99	В
	MOTA	2931	CG	ASP	59	61.807	-22.681	62.338	1.00 52.10	В
	MOTA.	2932	OD1	ASP	59	62.005	-23.464	61.385	1.00 51.56	В
	ATOM	2933		ASP	59		-22.987	63.525	1.00 52.60	В
45	MOTA	2934	С	ASP	59		-22.110	62.338	1.00 49.40	В
45	MOTA	2935	0	ASP	59	58.742	-23.315	62.197	1.00 48.84	В
	ATOM	2936	N	LYS	60	58.267	-21.404	63.256	1.00 47.59	В
	MOTA	2937	CA	LYS	60		-22.021	64.208	1.00 46.47	В
	ATOM	2938	CB	LYS	60		-22.949	65.114	1.00 45.88	В
50	MOTA	2939	CG.	LYS	60		-23.470	66.345	1.00 44.88	В
50	MOTA	2940	CD	LYS	60	58.462	-24.217	67.209	1.00 45.79	В
	MOTA	2941	CE	LYS	60	57.868	-24.729	68.503	1.00 47.18	В
	MOTA	2942	NZ	LYS	60	58.938	-25.298	69.384	1.00 48.54	В
	ATOM	2943	C	LYS	60		-20.862	64.977	1.00 45.74	В
		2944					-20.002			
55	MOTA		0.	LYS	60			65.532	1.00 45.66	В
22	MOTA	2945	N	SER	61		-20.802	64.999	1.00 44.14	В
	MOTA	2946	CA	SER	61	54.750	-19.718	65.697	1.00 42.32	В
	MOTA	2947	CB	SER	61	54.900	-18.419	64.892	1.00 43.45	В
	MOTA	2948	OG	SER	61		-18.594	63.545	1.00 42.02	В.
60	MOTA	2949	C	SER	61		-19.931	65.980	1.00 40.98	В
60	MOTA	2950	0	SER	61		-20.939	65.613	1.00 40.30	В
	ATOM	2951	N	SER	62	52.686	-18.954	66.669	1.00 40.63	В
	MOTA	2952	CA	SER	62		-18.944	66.992	1.00 38.79	В
	ATOM	-2953	СВ	SER	62		-18.549	.68.445	1.00 38.80	В
65	MOTA	2954	OG	SER	62		-19.441	69.325	1.00 38.30	В
65	MOTA	2955	С	SER	62		-17.862	66.115	1.00 37.30	В
	MOTA	2956	0	SER	62	51.293	-16.906	65.728	1.00 37.14	В
	MOTA	2957	N	ARG	63		-18.018	65.783	1.00 36.69	В
	ATOM	2958	CA	ARG	63		-17.017	64.959	1.00 35.86	
										В
70	MOTA	2959	СВ	ARG	63		-17.318	63.453	1.00 35.76	В
70	MOTA	2960	CG	ARG	63		-17.378	62.918	1.00 36.93	В
	ATOM	2961	CD	ARG	63	50.303	-17.660	61.418	1.00 38.47	В
	MOTA	2962	NE.	ARG	63		-16.499	60.608	1.00 40.73	В
	MOTA	2963	CZ	ARG	63	50.005	-15.428	60.393	1.00 40.83	В

	ATOM	2964	NH1	ARG	63	51.896	-15.353	60.928	1.00 41.75	В
	MOTA	2965	NH2		63		-14.433	59.629	1.00 40.58	В
	MOTA	2966	C	ARG	63		-16.982	65.296	1.00 34.60	В
_	MOTA	2967	0	ARG	63		-17.920	65.855	1.00 33.92	В
5	MOTA	2968	N	LYS	64	46.578	-15.865	64.968	1.00 33.48	В
	ATOM .	2969	CA	LYS	64	45.158	-15.676	65.193	1.00 31.00	В
	ATOM	2970	CB	LYS	64	44.913	-14.444	66.056	1.00 34.47	В
	ATOM	2971	CG	LYS	64		-14.581	67.508	1.00 36.74	В
	ATOM	2972	CD	LYS	64		-15.378	68.279	1.00 38.57	В
10										
10	ATOM	2973	CE	LYS	64		-15.324	69.773	1.00 39.71	В
	MOTA	2974	NZ	LYS	64	_	-15.964	70.596	1.00 40.02	B
	MOTA	2975	С	LYS	64		-15.428	63.805	1.00 29.35	В
	MOTA	2976	0	LYS	64	45.114	-14.604	63.045	1.00 29.23	В
	MOTA	2977	N	THR	65	43.537	-16.156	63.470	1.00 27.29	В -
15	ATOM	2978	CA	THR	65	42.917		62.165	1.00 24.96	В
	ATOM	2979	CB	THR	65		-17.321	61.338	1.00 24.86	В
	MOTA	2980	OG1	THR	65	44.442	-17.701	61.294	1.00 24.93	В
							-17.120			
	MOTA	2981	CG2		65			59.912	1.00 25.70	В
വറ	MOTA	2982	C	THR	65		-15.688	62.319	1.00 22.74	В
20	MOTA	2983	0	THR	65		-16.313	63.095	1.00 23.83	В
	ATOM	2984	N	TYR	66	40.999	-14.677	61.579	1.00 21.85	В
	ATOM '	2985	CA	TYR	66	39.601	-14.232	61.612	1.00 20.45	В
	MOTA	2986	CB	TYR	66	39.480	-12.844	62.234	1.00 18.74	В
	ATOM	2987	CG	TYR	66	40.144	-12.695	63.581	1.00 19.02	В
25	ATOM	2988		TYR	66	41.524	-12.584	63.695	1.00 18.23	В
	ATOM	2989		TYR	66		-12.420	64.946	1.00 19.22	. в
	MOTA	2990				39.387	-12.641		1.00 20.12	
				TYR	66			64.748		В
	ATOM	2991	CE2	TYR	66	39.986	-12.474	66.009	1.00 19.66	В
20 `	MOTA	2992	CZ	TYR	66		-12.367	66.109	1.00 20.40	В
30	MOTA	2993	ОН	TYR	66	41.915	-12.234	67.382	1.00 20.35	В
	ATOM	2994	С	TYR	66	39.027	-14.136	60.195	1.00 22.62	В
	ATOM	2995	0	TYR	66	39.736	-13.786	59.237	1.00 22.83	В
	ATOM	2996	N	THR	67 -		-14.464	60.058	1.00 22.62	В
	ATOM	2997	CA	THR	67		-14.424	58.755	1.00 23.36	B
35	ATOM	2998	CB	THR	67		-15.723	58.489	1.00 24.24	В.
55										
	MOTA	2999	0G1	THR	67		-16.854	58.576	1.00 26.83	В
	MOTA	3000	CG2	THR	67		-15.702	57.115	1.00 25.09	В
	MOTA	3001	С	THR	67		-13.241	58.669	1.00 23.25	В
in	MOTA	3002	0	THR	67	35.383	-12.979	59.598	1.00 23.74	В
40	ATOM	3003	N	PHE	68	36.199	-12.521	57.556	1.00 22.27	В
	MOTA	3004	CA	PHE	68	35.322	-11.379	57.354	1.00 23.47	В
	MOTA	3005	CB	PHE	68	36.108	-10.068	57.414	1.00 25.18	В
	MOTA	3006	CG	PHE	68	36.688	-9.788	58.758	1.00 28.91	В
	MOTA	3007		PHE	68		-10.407	59.162	1.00 31.76	В
45	ATOM	3008		PHE						
73					68	36.028	-8.957	59.655	1.00 30.45	В
	MOTA	3009		PHE	68		-10.211	60.444	1.00 33.13	В
	MOTA	3010	CE2	PHE	68	36.539	-8.749	60.947	1.00 32.68	В
	MOTA	3011	cz	PHE	68	37.733	-9.381	61.346	1.00 34.40	В
	MOTA	3012	С	PHE	68	34.664	~11.530	56.001	1.00 23.18	В
50	ATOM	3013	0	PHE	68	34.904	-12.505	55.318	1.00 23.09	В
	MOTA	3014	N	ASP	69	33.836	-10.560	55.625	1.00 22.35	В
	MOTA	3015	CA	ASP	69	33.127	-10.585	54.350	1.00 23.38	В
	MOTA	3016	CB	ASP	69	31.988	-9.559	54.386	1.00 23.05	В
	MOTA	3017	CG	ASP	69	30.917	-9.915	55.427	1.00 23.94	В
55	MOTA	3018		ASP	69	30.875	-9.341	56.538	1.00 21.68	В
33	ATOM	3019		ASP	69					
				-			-10.812	55.138	1.00 25.46	В
	ATOM	3020	C	ASP	69	34.071	-10.363	53.173	1.00 24.90	В
	MOTA	3021	0	ASP	69		-10.931	52.082	1.00 25.83	В
~	ATOM	3022	N	MET	70	35.089	-9.539	53.405	1.00 25.78	В
60	ATOM	3023	CA	MET	70	36.112	-9.233	52.412	1.00 26.18	В
	ATOM	3024	CB	MET	70	35.686	-8.073	51.517	1.00 27.89	В
	ATOM	3025	CG	MET	70	34.538	-8.363	50.564	1.00 29.68	В
	MOTA	3026	SD	MET	70	34.155	-6.927	49.495	1.00 34.95	В
	ATOM	3027	CE	MET	70	32.418	-7.227	49.126	1.00 32.58	· B
65	MOTA	3028	C	MET	70 70	37.378			1.00 32.58	
55							-8.801	53.150		В
	MOTA	3029	0	MET	70	37.301	-8.187	54.206	1.00 26.04	В
	MOTA	3030	N	VAL	71	38.540	-9.119	52.596	1.00 24.01	В
	MOTA	3031	CA	VAL	71	39.789	-8.724	53.228	1.00 23.4B	В
70	MOTA	3032	CB	VAL	71	40.496	-9.917	53.902	1.00 24.24	В
70	ATOM	3033	CG1	VAL	71	39.668	-10.429	55.086	1.00 23.32	В
	ATOM	3034		VAL	71	40.726	-11.004	52.882	1.00 24.53	В
	MOTA	3035	С	VAL	71	40.709	-8.121	52.181	1.00 23.86	В
	ATOM	3036	ō	VAL	71	40.841	-8.641	51.068	1.00 22.79	B
			-				J			

•	MOTA	3037	N	PHE	72	41.356	-7.025	52.551	1.00 22.62	В
	ATOM	3038	CA	PHE	72	42.229	-6.344	51.628	1.00 22.70	В
	MOTA	3039	CB	PHE	72	41.710	-4.936	51.321	1.00 20.63	В
	ATOM	3040	CG	PHE	72	40.318	-4.910	50.753	1.00 18.35	В
5	MOTA	3041		PHE	72	40.056	-5.419	49.493	1.00 15.95	В
-	ATOM	3042		PHE	72	39.261	-4.409	51.495	1.00 17.50	В
	ATOM	3043		PHE	72	38.771				
							-5.435	48.986	1.00 16.14	В
•	MOTA	3044		PHE	72	37.976	-4.425	50.985	1.00 17.48	В
10	MOTA	3045	CZ	PHE	72	37.732	-4.939	49.729	1.00 16.21	В
10	ATOM	3046	С	PHE	72	43.626	-6.197	52.178	1.00 22.69	В
	ATOM	3047	۰0	PHE	72	43.836	-5.523	53.181	1.00 22.50	В
	MOTA	3048	N	GLY	73	44.578	-6.837	51.508	1.00 22.82	В
	MOTA	3049	CA	GLY	73	45.965	-6.741	51.920	1.00 23.34	В
	MOTA	3050	C	GLY	73	46.584	-5.398	51.571	1.00 23.29	B
15	ATOM	3051	ŏ	GLY	73	45.982			1.00 23.23	
13							-4.561	50.885		В
	ATOM	3052	N	ALA	74	47.809	-5.199	52.037	1.00 23.40	В
	MOTA	3053	CA	ALA	74	48.531	-3.960	51.808	1.00 25.70	В
	MOTA	3054	CB	ALA	74	49.891	-4.016	52.523	1.00 25.78	В
aa .	MOTA	3055	С	ALA	74	48.725	-3.639	50.328	1.00 26.16	В
20	MOTA	3056	0	ALA	74	49.129	-2.556	49.978	1.00 27.50	. В
	ATOM	3057	N	SER	75	48.406	-4.584	49.459	1.00 27.00	В
	ATOM	3058	CA	SER	75	48.590	-4.358	48.031	1.00 28.47	В
	ATOM	3059	CB	SER	75	48.982	-5.679	47.335	1.00 28.85	В.
	ATOM	3060	OG	SER	75	48.019	-6.709	47.507	1.00 27.19	·B
25	ATOM	3061	c	SER	75	47.389	-3.728	47.319		
									1.00 27.90	В
	ATOM	3062	0	SER	75 26	47.542	-3.123	46.243	1.00 29.21	В
	MOTA	3063	N	THR	76	46.206	-3.853	47.918	1.00 26.99	В
	MOTA	3064	CA	THR	76 .	44.984	-3.315	47.320	1.00 25.45	В
20	MOTA	3065	CB	THR	76	43.746	-3.663	48.183	1.00 23.54	• в
30	ATOM	3066	0G1	THR	76	44.015	-3.345	49.545	1.00 23.44	В
	MOTA	3067	CG2	THR	76	43.436	-5.132	48.116	1.00 24.38	В
	MOTA	3068	С	THR	76	45.034	-1.803	47.087	1.00 25.69	В
•	MOTA	3069	ō	THR	76	45.543	-1.041	47.922	1.00 27.74	В
	ATOM	3070	N	LYS	77	44.507	-1.372	45.948	1.00 24.67	B
35	MOTA	3071	CA	LYS	ว่า	44.496			1.00 23.51	
55	MOTA						0.044	45.619		В
•		3072	CB	LYS	77	44.804	0.234	44.133	1.00 25.56	В
	MOTA	3073	CG	LYS	77	46.192	-0.249	43.719	1.00 28.23	В
	MOTA	3074	CD	LYS	77		0.132	42.209	1.00 31.78	В
40	MOTA	3075	CE	LYS	77	47.770	-0.560	41.784	1.00 33.69	В
40	MOTA	3076	NZ	LYS	77	47.942	-0.449	40.311	1.00 35.35	В
	MOTA	3077	С	LYS	77	43.150	0.677	45.956	1.00 21.23	В
	ATOM	3078	0	LYS	77	42.175	-0.023	46.154	1.00 19.65	В
	ATOM	3079	N	GLN	78	43.105	2.008	46.021	1.00 20.16	В
	ATOM	3080	CA	GLN	78	41.853	2.714	46.335	1.00 18.91	В
45	ATOM	3081	CB	GLN	78	42.004	4.226			
73	ATOM							46.179	1.00 18.69	В
		3082	CG	GLN	78	43.063	4.851	47.064	1.00 18.42	В
	ATOM	3083	CD	GLN	78	42.618	4.962	48.498	1.00 17.41	В
	ATOM	3084		GLN	. 78	42.152	3.997	49.085	1.00 20.11	В
50	MOTA	3085	NE2	GLN	78	42.756	6.143	49.066	1.00 14.62	В
50	MOTA	3086	С	GLN	78	40.743	2.294	45.377	1.00 19.40	В
	MOTA	3087	0	GLN	· 78	39.609	2.059	45.788	1.00 20.13	В
	MOTA	3088	N	ILE	79	41.074	2.208	44.092	1.00 17.68	В
	MOTA	3089	CA	ILE	79	40.089	1.815	43.094	1.00 15.86	В
	MOTA	3090	CB	ILE	79	40.727	1.779	41.678	1.00 15.34	В
55	ATOM	3091		ILE	79	41.709	0.597	41.561	1.00 16.93	В
-	ATOM	3092		ILE	79	39.640	1.641	40.612	1.00 14.82	В
					79					
	MOTA	3093		ILE		38.766	2.868	40.410	1.00 13.32	В
	MOTA	3094	C	ILE	79	39.463	0.440	43.399	1.00 14.58	В
60	MOTA	3095	0	ILE	79	38.304	0.217	43.130	1.00 15.24	В
60 ·	MOTA	3096	N	ASP	80	40.231	-0.479	43.969	1.00 13.09	В
	MOTA	3097	CA	ASP	80	39.683	-1.802	44.258	1.00 12.77	В
	MOTA	3098	СВ	ASP	80	40.800	-2.818	44.435	1.00 14.43	В
	ATOM	3099	CG	ASP	80	41.645	-2.953	43.204	1.00 18.24	В
	ATOM	3100	OD1		80	41.072	-2.882	42.088	1.00 18.24	В
65	ATOM	3101		ASP	80	42.874	-3.140	43.363		
55									1.00 21.75	В
	ATOM	3102	C	ASP	80	38.787	-1.829	45.487	1.00 12.00	В
	MOTA	3103	0	ASP	80	37.878	-2.638	45.590	1.00 10.17	В
	MOTA	3104	N	VAL	81	39.063	-0.938	46.430	1.00 11.87	В
70	MOTA	3105	CA	VAL	81	38.261	-0.841	47.638	1.00 10.20	В
70	MOTA	3106	CB	VAL	81	38.881	0.128	48.642	1.00 9.09	В
	MOTA	3107	CG1	VAL	81	37.857	0.529	49.689	1.00 7.52	. В
	ATOM	3108		VAL	81	40.071	-0.534	49.299	1.00 11.81	В
	ATOM	3109	C.	VAL	81	36.915	-0.292	47.224	1.00 10.85	В
										_

	MOTA	3110	0	VAL	81	35.879	-0.728	47.697	1.00 11.76	В
	ATOM	3111	Ň	TYR	82	36.948	0.681	46.326	1.00 12.12	В
	ATOM	3112	CA	TYR	82	35.735	1.304	45.845	1.00 13.85	В
_	ATOM	3113	CB	TYR	82	36.090	2.534	45.015	1.00 15.89	В
5	MOTA	3114	CG	TYR	82	34.870	3.259	44.530	1.00 18.66	В
	MOTA	3115		TYR	82	34.364	3.029	43.256	1.00 20.38	B
	MOTA	3116		TYR	82	33.201	3.645	42.824	1.00 22.59	В
	MOTA	3117		TYR	82	34.184	4.132	45.369	1.00 19.71	В
10	MOTA	3118		TYR	82	33.019.	4.755	44.953	1.00 22.44	В
10	MOTA MOTA	3119 3120	CZ OH	TYR	82	32.531	4.508	43.675	1.00 23.44	В
	MOTA	3121	C	TYR TYR	82 82	31.372 34.840	5.125 0.350	43.254 45.044	1.00 25.79 1.00 14.77	B B
	ATOM	3122	ō	TYR	82	33.635		45.331	1.00 13.77	В
	ATOM	3123	Ň	ARG	83	35.408	-0.299	44.035	1.00 15.58	В
15	MOTA	3124	CA	ARG	83	34.632	-1.236	43.220	1.00 18.14	В
	MOTA	3125	CB	ARG	83	35.517	-1.815	42.103	1.00 20.58	В
	MOTA	3126	CG	ARG	83	35.715	-0.868	40.915	1.00 23.85	. В
	MOTA	3127	CD	ARG	83	36.998	-1.162	40.161	1.00 26.52	В
20	MOTA	3128	NE	ARG	83	36.971	-2.428	39.436	1.00 30.77	В
20	MOTA	3129	CZ	ARG	83	36.255	-2.656	38.335	1.00 33.35	В
	ATOM ATOM	3130 3131	NH1 NH2	ARG	83 83	35.485 36.339	-1.703 -3.833	37.818 37.727	1.00 33.79	В
	ATOM	3132	C	ARG	83	34.009	-2.382	44.045	1.00 33.17 1.00 18.55	B B
	MOTA	3133	ŏ	ARG	83	32.867	-2.765	43.834	1.00 19:46	В
25	ATOM	3134	N	SER	84	34.764	-2.930	44.985	1.00 17.88	. В
	ATOM	3135	CA	SER	84	34.248	-4.009	45.809	1.00 17.71	В
	ATOM	3136	CB .	SER	84	35.380	-4.764	46.509	1.00 20.38	В
	MOTA	3137	OG	SER	84	36.282	-5.324	45.575	1.00 25.36	В
20	ATOM	3138	C	SER	84	33.298	-3.551	46.913	1.00 16.07	В
30	ATOM	3139	0	SER	84	32.241	-4.113	47.073	1.00 15.35	В
	MOTA	3140	N	VAL	85 85	33.685	-2.526	47.673	1.00 15.30	В
	MOTA MOTA	3141 3142	CA CB	VAL VAL	85 85	32.865 33.738	-2.048	48.795	1.00 14.98	В
	ATOM	3143		VAL	85	32.849	-1.521 -1.183	49.963 51.129	1.00 15.00 1.00 15.00	B B
35	ATOM	3144	CG2		85	34.775	-2.556	50.383	1:00 15.18	В.
	ATOM	3145	c	VAL	85	31.828	-0.960	48.509	1.00 14.85	В
	ATOM	3146	0	VAL	85	30.652	-1.162	48.734	1.00 13.96	В
	MOTA	3147	N	VAL	86	32.283	0.184	48.008	1.00 16.21	В
40	MOTA	3148	CA	VAL	86	31.409	1.313	47.740	1.00 15.47	В
40	ATOM	3149	СВ	VAL	86	32.205	2.597	47.571	1.00 15.27	В
	MOTA	3150	CG1	VAL	86	31.296	3.776	47.800	1.00 15.63	В
	ATOM ATOM	3151 3152		VAL	86	33.379	2.614	48.541	1.00 16.09	В
	ATOM	3153	0	VAL VAL	86 86	30.478 29.295	1.191 1.506	46.548 46.680	1.00 15.77 1.00 15.71	В В
45	ATOM	3154	N	CYS	87	30.976	0.734	45.399	1.00 15.71	В
-	ATOM	3155	CA	CYS	87	30.121	0.629	44.218	1.00 17.14	В
	MOTA	3156	CB	CYS	87	30.787	-0.168	43.108	1.00 16.23	В
	MOTA	3157	SG	CYS	87	30.003	0.173	41.511	1.00 22.71	В
50	MOTA	3158	С	CYS	87	28.753	-0.001	44.488	1.00 18.54	В
50	MOTA	3159	0	CYS	87	27.752	0.494	44.050	1.00 19.06	В
	MOTA MOTA	3160	И	PRO	88	28.707	-1.117	45.207	1.00 20.44	В
	ATOM	3161 3162	CD CA	PRO PRO	88 88	29.827 27.422	-2.005	45.536	1.00 22.48	В
	ATOM	3163	CB	PRO	88	27.847	-1.759 -3.060	45.507 46.157	1.00 21.26	B B
55	ATOM	3164	CG	PRO	88	29.168	-3.337	45.512	1.00 22.69	В
	ATOM	3165	c	PRO	88	26.542	-0.890	46.434	1.00 22.59	В
	MOTA	3166	0	PRO	88	25.333	-0.797	46.254	1.00 22.78	В
	MOTA	3167	N	ILE	89	27.151	-0.273	47.446	1.00 22.51	В
40	MOTA	3168	CA	ILE	89	26.409	0.582	48.388	1.00 22.44	В
60	MOTA	3169	СВ	ILE	89	27.298	1.003	49.579	1.00 22.87	В
	MOTA	3170	CG2		89	26.592	2.040	50.408	1.00 22.27	В
	MOTA	3171	CG1		89	27.607	-0.227	50.439	1.00 24.48	В
	MOTA MOTA	3172 3173	CD1	ILE	89 89	28.465 25.843	0.041 1.841	51.641 47.727	1.00 26.67	В
65	ATOM	3174	ò	ILE	89	24.734	2.264	48.035	1.00 22.09 1.00 21.69	. B B
	ATOM	3175	N	LEU	90	26.607	2.450	46.829	1.00 21.87	В
	ATOM	3176	CA	LEU	90	26.122	3.640	46.157	1.00 23.17	В
	ATOM	3177	СВ	LEU	90	27.195	4.228	45.243	1.00 20.80	В
- 0	MOTA	3178	CG	LEU	90	26.773	5.485	44.498	1.00 18.97	B
70	MOTA	3179	CD1	LEU	90	26.169	6.492	45.446	1.00 18.16	В
	MOTA	3180	CD2		90	27.987	6.053	43.822	1.00 20.13	В
	MOTA	3181	C	LEU	90	24.891	3.282	45.334	1.00 24.49	В
	MOTA	3182	0	LEU	90	23.963	4.091	45.207	1.00 24.70	В

•	MOTA	3183	N	ASP	91		24.887	2.068	44.781	1.00 25.50	В
	MOTA	3184	CA	ASP	91		23.765	1.617	43.975	1.00 26.54	В
	ATOM ATOM	3185 3186	CB	ASP	91		24.042	0.258	43.331	1.00 27.25	В
5	ATOM	3187	CG	ASP	91 91		24.841 24.725	0.373 1.424	42.045	1.00 29.15 1.00 28.90	B B
,	ATOM	3188		ASP	91		25.559	-0.601	41.701	1.00 29.60	В
	ATOM	3189	c	ASP	91		22.537	1.512	44.848	1.00 27.48	В
	MOTA	3190	ō	ASP	91		21.427	1.740	44.399	1.00 28.35	В
	MOTA	3191	N	GLU	92		22.736	1.185	46.115	1.00 28.27	В
10	MOTA	3192	CA	GLU	92		21.603	1.065	47.018	1.00 28.89	В
	MOTA	3193	CB	GLU	92		22.008	0.214	48.219	1.00 30.33	В
	MOTA	3194	CG	GLU	92		20.839		49.057	1.00 33.34	В
	MOTA	3195	CD	GLU	92		21.141	-1.578	49.772	1.00 35.27	В
15	MOTA	3196		GLU	92 92		20.340	-2.000	50.633	1.00 36.65	В
13	MOTA MOTA	3197 3198	C	GLU GLU	92		22.181 21.106	-2.200 2.459	49.469 47.424	1.00 35.05	B B
	ATOM	3199	ŏ	GLU	92		19.897	2.685	47.581	1.00 27.53	В
	MOTA	3200	N	VAL	93		22.037	3.395	47.585	1.00 27.17	В
	MOTA	3201	CA	VAL	93		21.663	4.757	47.938	1.00 26.25	В
20	MOTA	3202	CB	VAL	93		22,902	5.681	48.072	1.00 27.41	. В
	ATOM	3203		VAL	93		22.455	7.125	48.357	1.00 27.55	В
	ATOM	3204		VAL	93		23.807	5.170	49.178	1.00 29.02	В.
	MOTA	3205	Č	VAL	93		20.771	5.339	46.843	1.00 24.60	В
25	MOTA MOTA	3206 3207	0	VAL	93 94		19.759	5.955	47.110	1.00 24.17	·B
23	MOTA	3207	N CA	ILE	94		21.175 20.398	5.150 5.657	45.596 44.466	1.00 22.93 1.00 23.06	B B
	MOTA	3209	CB	ILE	94		21.193	5.441	43.130	1.00 23.00	В
	MOTA	3210		ILE	94		20:367	5.867	41.905	1.00 18.23	В
	ATOM	3211		ILE	94	•	22.498	6.262	43.205	1.00 20.00	. В
30	MOTA	3212	CD1	ILE	94		23.382	6.115	42.021	1.00 18.08	В
	ATOM	3213	С	ILE	94		18.984	5.036	44.384	1.00 23.71	В
	ATOM	3214	0	ILE	94		18.079	5.630	43.845	1.00 24.46	В
	ATOM	3215	N	MET	95		18.787	3.839	44.924	1.00 25.14	В
35 ⁻	ATOM ATOM	3216 3217	CA CB	MET MET	95 05		17.451	3.234	44.893	1.00 25.03	В
JJ	ATOM	3218	CG	MET	95 95		17.511 17.896	1.735 0.898	45.167 43.984	1.00 24.81 1.00 24.81	B B
•	ATOM	3219	SD	MET	95		17.840	-0.821	44.434	1.00 28.44	В
	ATOM	3220	CE	MET	95		19.568	-1.182	44.778	1.00 27.32	В
	ATOM	3221	C	MET	95		16.585	3.864	45.977	1.00 25.84	В
40	ATOM	3222	0	MET	95		15.407	3.606	46.068	1.00 26.55	В
	ATOM	3223	N	GLY	96		17.193	4.694	46.811	1.00 26.29	В
	MOTA	3224	CA	GLY	96		16.417	5.335	47.854	1.00 26.67	В
	MOTA	3225	C	GLY	96		16.650	4.824	49.264	1.00 28.04	В
45	ATOM ATOM	3226 3227	N N	GLY TYR	96 97		15.864 17.733	5.121 4.075	50.170 49.454	1.00 29.08 1.00 28.81	B B
	ATOM	3228	CA	TYR	97		18.081	3.524	50.760	1.00 29.52	В
	ATOM	3229	СВ	TYR	97		18.680	2.117	50.591	1.00 31.73	В
	ATOM	3230	CG	TYR	97		17.674	1.041	50.230	1.00 34.37	В
~^	MOTA	3231	CD1	TYR	97		17.016	0.310	51.223	1.00 35.37	В
50	ATOM	3232		TYR	97		16.087	-0.663	50.904	1.00 36.70	В
	ATOM	3233		TYR	97		17.370	0.769	48.901	1.00 35.61	В
	MOTA	3234		TYR	97		16.439	-0.198	48.569	1.00 37.43	В
	MOTA MOTA	3235 3236	CZ OH	TYR TYR	97 97		15.800 14.858	-0.909 -1.862	49.575 49.257	1.00 38.91	В
55	ATOM	3237	C	TYR	97		19.090	4.391	51.528	1.00 28.25	B B
	ATOM	3238	ō	TYR	97		19.819	5.172	50.943	1.00 29.03	В
	MOTA		N	ASN	98		19.107	4.266		1.00 26.29	В
	ATOM	3240	CA	ASN	98		20.087	4.993	53.646	1.00 24.16	В
C 0	MOTA	3241	CB	ASN	98		19.520	5.396	54.994	1.00 23.70	В
60 ·	MOTA	3242	CG	asn	98		18.552	6.526	54.883	1.00 21.81	В
	MOTA	3243		ASN	98		18.764	7.475	54.138	1.00 20.22	В
	MOTA	3244		ASN	98		17.483	6.442	55.642	1.00 22.90	В
	ATOM ATOM	3245 3246	c	ASN	98 98		21.262	4.051	53.883	1.00 22.53	В
65	MOTA	3240	O N	ASN CYS	98		21.076 22.475	2.860 4.573	54.149 53.770	1.00 23.91 1.00 20.08	B B
	ATOM	3248	CA	CYS	99		23.652	3.741	53.776	1.00 20.08	В
	MOTA	3249	CB	CYS	99		24.239	3.318	52.641	1.00 16.30	В
	MOTA	3250	SG	CYS	99		23.128	2.271	51.748	1.00 16.76	. B
70	MOTA	3251	С	CYS	99		24.717	4.437	54.786	1.00 13.97	В
70	ATOM	3252	0	CYS	99		24.764	5.664	54.867	1.00 13.48	В
	MOTA	3253	N	THR	100		25.584	3.631	55.374	1.00 12.82	В
	MOTA	3254	CA	THR	100		26.646	4.149	56.209	1.00 10.88	В
	MOTA	3255	CB	THR	100		26.177	4.209	57.660	1.00 9.58	В

	MOTA	3256	001	THR	100	25.155	5.204	57.768	1.00 6.29	ъ
									-	В
	ATOM	3257	CG2	THR	100	27.327	4.524	58.590	1.00 10.26	В
	MOTA	3258	С	THR	100	27.874	3.264	56.104	1.00 10.53	. в
_	MOTA	3259	0	THR	100	27.764	2.056	56.040	1.00 10.24	В
5	ATOM	3260	N	ILE	101	29.044	3.890	56.059	1.00 10.89	В
	ATOM	3261	CA	ILE	101		3.156			
						30.303		55.993	1.00 12.11	В
	MOTA	3262	CB	ILE	101	31.004	3.297	54.642	1.00 13.63	В
	MOTA	3263	CG2	ILE	101	32.258	2.424	54.623	1.00 13.65	В
	MOTA	3264	CG1	ILE	101	30.057	2.935	53.504	1.00 15.35	В
10										
10	MOTA	3265	CD1	ILE	101	30.607	3.332	52.135	1.00 15.19	В
	MOTA	3266	С	ILE	101	31.226	3.776	57.027	1.00 11.10	В
	MOTA	3267	0	ILE	101	31.518	4.944	56.962		
									1.00 13.95	В
	ATOM	3268	N	PHE	102	31.690	2.961	57.960	1.00 8.97	В
	ATOM	3269	CA	PHE	102	32.569	3.412	59.024	1.00 5.36	
15										В
13	MOTA	3270	CB	PHE	102 .	32.254	2.693	60.337	1.00 5.27	В
	ATOM	3271	CG	PHE	102 .	30.964	3.097	60.979	1.00 3.08	В
	MOTA	3272	CDI	PHE	102	30.912	4.233	61.785	1.00 3.17	В
•	ATOM	3273	CD2	PHE	102	29.821	2.315	60.839	1.00 1.92	В
20	mota	3274		PHE	102	29.737	4.591	62.458	1.00 2.33	В
20	MOTA	3275	CE2	PHE	102	28.648	2.667	61.505	1.00 1.69	В
	ATOM	3276	CZ	PHE	102					
						28.608	3.812	62.323	1.00 1.17	В
	MOTA	3277	С	PHE	102	33.974	2.937	58.708	1.00 4.97	В
	MOTA	3278	0	PHE	102	34.160	1.984	57.997	1.00 6.23	В
^-	MOTA	3279	N	ALA	103	34.956	3.641	59.244	1.00 5.31	В
25	MOTA	3280	CA	ALA	103	36.345	3.256	59.091	1.00 3.70	- B
	MOTA	3281	CB	ALA	103	37.115	4.337	58.408	1.00 2.97	. В
	ATOM	3282	С	ALA	103	36.781	3.126	60.546	1.00 3.79	В
	MOTA	3283	0	ALA	103	36.811	4.105	61.266	1.00 4.80	В
	MOTA	3284	N	TYR	104	37.086	1.908	60.981	1.00 3.80	В
30										
50	MOTA	3285	CA	TYR	104	37.503	1.670	62.366	1.00 3.56	В
	MOTA	3286	CB	TYR	104	36.507	0.751	63.061	1.00 2.47	В
	ATOM		CG							
		3287		TYR	104	36.842	0.498	64.507	1.00 1.59	В
	MOTA	3288	CD1	TYR	104.	37.780	-0.465	64.875	1.00 1.99	В
	MOTA	3289		TYR	104	38.079	-0.706	66.227		
35									1.00 1.00	В
<i>33</i>	MOTA	3290	CD2	TYR	104	36.211	1.215	65.510	1.00 3.23	В
	MOTA	3291	CE2	TYR	104	36.492	0.988	66.863	1.00 1.00	В
	MOTA	3292	CZ	TYR	104	37.419	0.031	67.217	1.00 1.00	В
	ATOM	3293	OH	TYR	104	37.667	-0.164	68.555	1.00 1.00	В
40	MOTA	3294	С	TYR	104	38.893	1.046	62.517	1.00 3.38	В
40	ATOM	3295	0	TYR	104	39.225	0.087	61.843	1.00 3.35	Ė
	MOTA	3296	N	GLY	105	39.680	1.586	63.440	1.00 4.31	В
	ATOM	3297	CA	GLY	105	41.024	1.088	63.646	1.00 5.04	В
	ATOM	3298	Ċ	GLY	105					
						41.931	2.086	64.335	1.00 5.61	В
	ATOM	3299	0	GLY	105	41.560	3.226	64.565	1.00 5.55	В
45	MOTA	3300	N	GLN	106	43.132	1.627	64.657		
7.5									1.00 7.21	В
	MOTA	3301	CA	GLN	106	44.154	2.414	65.338	1.00 9.77	В
	MOTA	3302	CB	GLN	106	45.303	1.473	65.701	1.00 11.84	В
	MOTA	3303	CG	GLN	106	46.625	2.127	65.977	1.00 18.02	В
	MOTA	3304	CD	GLN	106	47.651	1.110	66.407	1.00 20.93	В
50										
50	MOTA	3305	OE1	GLN	106	47.887	0.126	65.707	1.00 20.58	В
	MOTA	3306	NE2	GLN	106	48.265	1.333	67.569	1.00 24.16	В
	MOTA	3307	С	GLN	106	44.684	3.603	64.525		
										В
	ATOM	3308	0	GLN	106	44.759	3.535	63.318	1.00 8.64	В
	ATOM	3309	N	THR	107	45.040	4.693	65.206	1.00 9.25	В
55										
J J	MOTA	3310	CA	THR	107	45.589	5.863	64.537	1.00 9.91	В
	MOTA	3311	CB	THR	107	46.090	6.935	65.545	1.00 11.30	В
		3312								
	MOTA			THR	107	44.998	7.433	66.328	1.00 12.57	В
	MOTA	3313	CG2	THR	107	46.715	8.089	64.807	1.00 11.37	В
	ATOM	3314	C	THR	107		5.384	63.720		
60						46.784			1.00 9.43	В
60	MOTA	3315	0	THR	107	47.631	4.615	64.226	1.00 6.62	В
	MOTA	3316	N	GLY	108	46.836	5.797	62.455	1.00 7.40	
										В
	MOTA	3317	CA	GLY	108	47.956	5.419	61.613	1.00 7.87	В
	MOTA	3318	С	GLY	108	47.801	4.136	60.815	1.00 7.55	
										В
	MOTA	3319	0	GLY	108	48.771	3.609	60.263	1.00 10.21	. в
65	MOTA	3320	N	THR	109	46.581	3.624	60.748	1.00 5.82	В
	ATOM	3321	CA	THR-	109	46.349	2.400	59.992	1.00 4.83	В
	ATOM	3322	CB	THR	109	45.588	1.329	60.827	1.00 3.30	В
	ATOM	3323	OG1							
					109	44.316	1.824	61.248	1.00 2.94	В
	MOTA	3324	CG2	THR	109	46.388	0.954	62.027	1.00 4.86	В
70	MOTA	3325	C	THR	109	45.611	2.616	58.675		
									1.00 5.10	В
	MOTA	3326	0	THR	109	45.305	1.648	57.954	1.00 5.03	В
	ATOM	3327	N	GLY	110	45.298	3.871	58.364		
									1.00 3.29	В
	MOTA	3328	CA	GLY	110	44.613	4.141	57.122	1.00 1.90	В

	MOTA	3329	С	GLY	110	43.131	4.484	57.097	1.00 2.61	В
	MOTA	3330	0	GLY	110	42.521	4.385	56.025	1.00 1.00	В
	ATOM	3331	N	LYS	111	42.539	4.885	58.227	1.00 4.13	В
_	MOTA	3332	CA	LYS	111	41.117	5.282	58.231	1.00 2.65	В
5	MOTA	3333	CB	LYS	111	40.636	5.636	59.651	1.00 2.73	В.
	MOTA	3334	CG	LYS	111	40.588	4.463	60.630	1.00 4.22	В
	MOTA	3335	CD	LYS	111	39.990	4.860	61.974	1.00 1.25	B
	MOTA	3336	CE	LYS	111	40.770	5.978	62.652	1.00 1.64	В
10	MOTA	3337	NZ	LYS	111	42.112	5.563	63.122	1.00 3.15	В
10	MOTA	3338	С	LYS	111	40.876	6.516	57.319	1.00 3.52	В
	MOTA	3339	.0	LYS	111	39.940	6.553	56.504	1.00 3.17	В
	MOTA	3340	N	THR	112	41.738		57.421	1.00 2.71	В
	MOTA	3341	CA	THR	112	41.536	8.697	56.607	1.00 4.38	В
1 5	MOTA	3342	CB	THR	112	42.245	9.927	57.209	1.00 3.24	В
15	MOTA	3343	0G1		112	41.689	10.219	58.500	1.00 2.46	В
	MOTA	3344	CG2		112	42.049	11.122	56.306	1.00 5.02	В
	MOTA	3345	C	THR	112	42.010	8.459	55.175	1.00 6.62	В
	MOTA	3346	0	THR	112	41.499	9.074	54.223	1.00 5.92	В
20	MOTA	3347	N	PHE	113	42.974	7.556	55.013	1.00 7.30	В
20	MOTA MOTA	3348 3349	CB	PHE	113 113	43.484 44.690	7.275 6.342	53.680 53.705	1.00 9.51 1.00 11.02	B B
	ATOM	3350	CG	PHE	113	45.299	6.119	52.344	1.00 11.02	В
	ATOM	3351		PHE	113	46.106	7.088	51.763	1.00 13.42	В.
	ATOM	3352		PHE	113	45.021	4.974	51.624	1.00 13.65	·B
25	MOTA	3353		PHE	113	46.626	6.927	50.496	1.00 13.19	В
	ATOM	3354	CE2		113	45.542	4.806	50.345	1.00 14.93	B
	ATOM	3355	CZ	PHE	113	46.346	5.792	49.784	1.00 13.30	B
	MOTA	3356	C	PHE	113	42:393	6.604	52.866	1.00 10.02	В
	MOTA	3357	0	PHE	113	42.195	6.916	51.689	1.00 9.19	В
30	MOTA	3358	N	THR	114	41.686	5.686	53.519	1.00 9.92	В
	MOTA	3359	CA	THR	114	40.601	4.946	52.905	1.00 8.86	В
	MOTA	3360	CB	THR	114	40.157	3.792	53.812	1.00 9.97	В
	MOTA	3361	.0G1	THR	114	41.256	2.900	54.000	1.00 10.04	В
26.	ATOM	3362	CG2	THR	114	39.026	3.006	53.174	1.00 10.07	В
35	MOTA	3363	С	THR	114	39.397	5.824	52.608	1.00 8.06	В
	MOTA	3364	Ο.	THR	114	38.935	5.875	51.496	1.00 8.14	В
	MOTA	3365	N	MET	115	38.908	6.538	53.612	1.00 6.57	В
	MOTA	3366	CA	MET	. 115	37.730	7.365	53.422	1.00 6.18	В
40	MOTA	3367	CB	MET	115	37.149	7.844	54.760	1.00 8.16	В
40	ATOM	3368	CG	MET	115	36.761	6.723	55.717	1.00 12.31	В
	MOTA	3369 3370	SD	MET	115	35.709	5.494	54.920	1.00 17.76	В
	MOTA MOTA	3371	CE	MET MET	115 115	34.142 37.903	6.334 8.594	54.973 52.570	1.00 16.39 1.00 6.31	В
	ATOM	3372	ŏ	MET	115	36.998	8.943	51.837	1.00 6.31 1.00 10.20	B B
45	MOTA	3373	N	GLU	116	39.061	9.244	52.660	1.00 10.20	В
	ATOM	3374	CA	GLU	116	39.295	10.476	51.909	1.00 2.45	В
	ATOM	3375	СВ	GLU	116	39.743	11.607	52.838	1.00 2.23	В
	ATOM	3376	CG	GLU	116	38.737	11.962	53.924	1.00 1.00	B
	ATOM	3377	CD	GĽU	116	39.091	13.216	54.722	1.00 1.00	В
50	MOTA	3378	OE1	GLU	116	40.124	13.850	54.464	1.00 1.56	В
	MOTA	3379	OE2	GLU	116	38.323	13.586	55.626	1.00 1.00	В
	MOTA	3380	С	GLU	116	40.342	10.311	50.843	1.00 2.04	В
	MOTA	3381	0	GLU	116	40.070	10.587	49.695	1.00 1.54	В
e e	MOTA	3382	N	GLY	117	41.539	9.869	51.235	1.00 2.71	В
55	MOTA	3383	CA	GLY	117	42.603	9.663	50.263	1.00 3.19	В
	MOTA	3384	C	GLY	117	43.531	10.842	50.294	1.00 1.91	В
	ATOM	3385	0	GLY	117	43.293		51.033		В
	ATOM	3386	N	GLU	118	44.568	10.822	49.466	1.00 3.14	В.
60 -	ATOM	3387	CA.	GLU	118	45.562	11.897	49.412	1.00 3.61	В.
00	ATOM	3388	CB	GLU	118	46.879	11.427	50.051	1.00 3.14	В
	MOTA	3389	CG	GLU	118	46.652	10.690	51.389	1.00 7.09	В
	ATOM ATOM	3390 3391	CD	GLU	118	47.933	10.200	52.062	1.00 9.57	В
	MOTA	3392		GLU GLU	118 118	48.831 48.030	9.748 10.259	51.317 53.317	1.00 11.82	В
65	MOTA	3393	·C	GLU	118	45.813	12.253	47.959	1.00 6.51 1.00 4.59	В
J.J	ATOM	3394	ō	GLU	118	45.209	11.670	47.063	1.00 4.33	B
	ATOM	3395	N	ARG	119	46.681	13.221	47.713	1.00 7.04	В
	ATOM	3396	CA	ARG	119	46.976	13.564	46.329	1.00 7.04	В
	ATOM	3397	СВ	ARG	119	47.171	15.067	46.131	1.00 10.32	В
70	ATOM	3398	CG	ARG	119	45.961	15.941	46.462	1.00 13.02	В
-	ATOM	3399	CD	ARG	119	44.705	15.414	45.837	1.00 13.25	B
	ATOM	3400	NE.	ARG	119	44.838	15.093	44.420	1.00 13.98	В
	ATOM	3401	CZ	ARG	119	44.759	15.955	43.411	1.00 11.43	В
					-				· · 	-

	MOTA	3402	NH1	ARG	119	44.543	17.247	43.614	1.00 9.13	В
	ATOM	3403	NH2	ARG	119	44.890	15.498	42.175	1.00 10.86	В
	MOTA	3404	С	ARG	119	48.274	12.907	45.912	1.00 12.67	В
	MOTA	3405	0	ARG	119	49.210	12.823	46.712	1.00 12.43	В
5	MOTA	3406	N	SER	120	48.328	12.416	44.675	1.00 15.44	В
	ATOM	3407	CA	SER	120	49.563	11.812	44.182	1.00 17.48	B
	ATOM	3408	CB	SER	120	49.392	11.272	42.755	1.00 18.24	В
	ATOM	3409	OG	SER	120	48.605	10.090	42.735	1.00 19.78	В
	ATOM	3410	c	SER	120	50.519	12.978	44.185	1.00 19.78	
10										В
10	MOTA	3411	0	SER	120	50.161	14.050	43.772	1.00 20.75	В
	MOTA	3412	N	PRO	121	51.748	12.782	44.660	1.00 20.06	В
	MOTA	3413	CD	PRO	121	52.403	11.508	45.013	1.00 20.52	В
	MOTA	3414	CA	PRO	121	52.700	13.896	44.686	1.00 20.89	В
1.5	ATOM	3415	CB	PRO	121	53.912	13.275	45.385	1.00 21.27	В
15	MOTA	3416	CG	PRO	121	53.881	11.834	44.872	1.00 21.35	В
	MOTA	3417	С	PRO	121	53.028	14.538	43.332	1.00 21.75	В
	MOTA	3418	0	PRO	121	52.835	13.918	42.270	1.00 21.17	·B
	MOTA	3419	N	ASN	122	53.514	15.785	43.393	1.00 21.50	В
	ATOM	3420	CA	ASN	122	53.957	16.561	42.227	1.00 22.52	В
20	MOTA	3421	CB	ASN	122	55.199	15.865	41.632	1.00 24.29	B
	MOTA	3422	CG	ASN	122	56.137	16.828	40.956	1.00 26.30	B
	ATOM	3423		ASN	122	56.538	17.815	41.553		B
	ATOM	3424		ASN	122	56.488	16.552	39.705	1.00 26.63	
	ATOM	3425		ASN	122					В
25			C			52.917	16.852	41.126	1.00 22.37	В
25	MOTA	3426	0	ASN	122 .	53.271	16.962	39.930	1.00 20.20	· B
	ATOM	3427	N	GLU	123	51.651	16.999	41.518	1.00 22.38	. В
	ATOM	3428	CA	GLU	123	50.573	17.294	40.561	1.00 22.86	В
	MOTA	3429	CB	GLU	123	50.664	18.735	40.072	1.00 21.58	В
30	MOTA	3430	CG	GLU	123	50.338	19.754	41.110	1.00 21.60	В
30	MOTA	3431	CD	GLU	123	50.218	21.112	40.506	1.00 23.71	В
	MOTA	3432	OE1		123	51.124	21.512	39.736	1.00 24.05	В
	MOTA	3433	OE2		123	49.220	21.789	40.808	1.00 24.70	В
	MOTA	3434	С	GLU	123.	50.573	16.401	39.319	1.00 23.43	В
25	MOTA	3435	0	GLU	123	50.357	16.856	38.189	1.00 22.15	8
35	MOTA	3436	N	GLU	124	50.809	15.116·	39.538	1.00 25.66	в.
	MOTA	3437	CA	GLU	124	50.840	14.186	38.435	1.00 27.17	В
	· ATOM	3438	CB	GLU	124	51.320	12.816	38.905	1.00 28.99	В
	MOTA	3439	CG	GLU	124	51.698	11.884	37.763		В
	MOTA	3440	CD	GLU	124	52.179	10.531	38.247	1.00 36.81	В
40	ATOM	3441		GLU	124	52.681	10.475	39.395	1.00 37.60	B
	MOTA	3442		GLU	124	52.061	9.543	37.476	1.00 36.71	В
	ATOM	3443	C.	GLU	124	49.466	14.045	37.791	1.00 26.54	В
	ATOM	3444	ō	GLU	124	49.351	13.966	36.571	1.00 28.04	В
	ATOM	3445	N	TYR	125	48.425	14.023	38.616	1.00 24.51	В
45	ATOM	3446	CA	TYR	125	47.065	13.864	38.117	1.00 22.37	В
	ATOM	3447	CB	TYR	125	46.424	12.570	38.618		
	ATOM	3448	CG	TYR	125	47.232	11.305		1.00 24.02	В
	MOTA	3449						38.445	1.00 24.34	В
				TYR	125	48.215	10.951	39.372	1.00 24.16	В
50	ATOM	3450		TYR	125	48.938	9.770	39.238	1.00 24.97	В
50	MOTA	3451	CD2		125	46.994	10.440	37.368	1.00 23.29	В
	MOTA	3452	CE2	TYR	125	47.715	9.257	37.224	1.00 23.28	В
	MOTA	3453	CZ	TYR	125	48.685	8.927	38.165	1.00 25.16	В
	MOTA	3454	ОН	TYR	125	49.395	7.750	38.059	1.00 24.88	В
E E	MOTA	3455	С	TYR	125	46.089	14.936	38.586	1.00 22.58	В
55	MOTA	3456	0	TYR	125	46.366	15.703	39.516	1.00 24.23	В
	MOTA	3457	N	THR	126	44.941	14.984	37.920	1.00 21.47	В
	MOTA	3458	CA	THR	126	43.889	15.919	38.280	1.00 20.00	В
	MOTA	3459	CB	THR	126	42.913	16.147	37.140	1.00 20.72	В
	MOTA	3460	OG1	THR	126	42.379	14.888	36.723	1.00 21.10	В
60	MOTA	3461	CG2		126	43.598	16.837	35.984	1.00 20.85	В
	MOTA	3462	С	THR	126	43.158	15.142	39.353	1.00 17.64	В
	ATOM	3463	ō	THR	126	43.223	13.940	39.359	1.00 16.55	B
	ATOM	3464	N	TRP	127	42.441	15.820	40.241	1.00 16.83	В
	ATOM	3465	CA	TRP	127	41.749	15.118	41.332	1.00 15.87	. в
65	ATOM	3466	CB	TRP	127	40.927	16.080	42.213	1.00 14.78	
70	ATOM	3467	CG	TRP	127					В
		3468				39.645	16.561	41.596	1.00 12.27	В
	MOTA		CD2		127	38.379	15.935	41.708	1.00 9.16	В
	ATOM .	3469	CE2		127	37.467	16.702	40.951	1.00 9.12	В
70	MOTA	3470	CE3		127	37.925	14.802	42.375	1.00 7.09	В
70	MOTA	3471	CD1		127	39.462	17.662	40.795	1.00 11.95	В
	MOTA	3472	NE1		127	38.150	17.749	40.405	1.00 11.09	В
	MOTA	3473	CZ2		127	36.142	16.366	40.845	1.00 8.67	В
	MOTA	3474	CZ3	TRP	127	36.606	14.472	42.271	1.00 7.96	В

	ATOM	3475	CH2	TRP	127		35.724	15.251	41.511	1.00 9.12	В
	ATOM	3476	C	TRP	127		40.824	13.969	40.917	1.00 15.77	В
	ATOM	3477	ŏ	TRP	127		40.807	12.907	41.536	1.00 16.78	В
_	MOTA	3478	N	GLU	128		40.065	14.145	39.855	1.00 16.83	В
5	ATOM	3479	CA	GLU	128		39.168	13.073	39.465	1.00 16.42	В
	MOTA	3480	CB	GLU	128		38.092	13.631	38.537	1.00 15.75	В
	MOTA	3481	CG	GLU	128	•	38.578	14.230	37.234	1.00 14.47	В
	MOTA	3482	CD	GLU	128		37.432	14.890	36.478	1.00 17.33	В
10	MOTA	3483		GLU	128		36.986	15.975	36.897	1.00 18.91	В
10	MOTA	3484		GLU	128		36.954	14.324	35.477	1.00 17.86	В
	MOTA	3485	·C	GLU	128		39.828	11.828	38.847	1.00 17.44	В
	MOTA MOTA	3486 3487	0	GLU	128		39.142	10.851	38.564	1.00 17.96	В
	ATOM	3488	N CA	GLU GLU	129 129		41.147 41.836	11.846	38.653 38.078	1.00 18.02	В
15	MOTA	3489	CB	GLU	129	•	42.509	10.692 11.020	36.740	1.00 19.12 1.00 20.74	В
	ATOM	3490	CG	GLU	129		41.574	11.402	35.595	1.00 26.16	B B
	ATOM	3491	CD	GLU	129		42.324	11.739	34.299	1.00 20.10	В
	ATOM	3492		GLU	129		41.711	12.357	33.393	1.00 32.49	В
	MOTA	3493		GLU	129		43.521	11.385	34.178	1.00 32.69	В
20	MOTA	3494	С	GLU	129		42.945	10.219	38.990	1.00 18.40	. В
	MOTA	3495	0	GLU	129		43.677	9.331	38.637	1.00 18.01	В
	MOTA	3496	N	ASP	130		43.051	10.816	40.173	1.00 17.65	В,
	ATOM	3497	CA	ASP	130		44.115	10.465	41.113	1.00 17.80	В
25	MOTA	3498	CB	ASP	130		44.200	11.536	42.211	1.00 17.64	·B
23	MOTA	3499	CG	ASP	130		45.540	11.556	42.908	1.00 19.83	В
	MOTA	3500		ASP	130		46.026	10.466	43.291	1.00 20.74	В
	MOTA MOTA	3501		ASP	130		46.097	12.661	43.070	1.00 20.64	. В
	ATOM	3502 3503	c o	ASP ASP	130 130		43.843 42.792	9.091	41.704 42.302	1.00 17.66	В
30	ATOM	3504	N	PRO	131		44.778	8.867 8.141	42.302	1.00 18.25 1.00 17.22	В
	ATOM	3505	CD	PRO	131		46.046	8.282	40.780	1.00 17.22	B B
	ATOM	3506	CA	PRO	131		44.617	6.778	42.052	1.00 16.05	В
•	ATOM	3507	CB	PRO	131		45.716	5.994	41.316	1.00 14.70	В
	MOTA	3508	CG	PRO	131		46.802	7.019	41.154	1.00 17.48	B
35	MOTA .	.3509	С	PRO	131		44.668	6.713	43.589	1.00 15.30	В
	MOTA	3510	0	PRO	131		44.318	5.697	44.187	1.00 14.37	В
	ATOM	3511	N	LEU	132		45.114	7.797	44.226	1.00 15.18	В
	MOTA	3512	CA	LEU				7.841	45.683	1.00 13.57	В
40	MOTA	3513	CB	LEU	132		46.380	8.644	46.165	1.00 12.21	В
70	MOTA MOTA	3514 3515	CG	LEU	132		47.741	8.012	45.842	1.00 12.83	В
	MOTA	3516		LEU	132 132		48.850 47.773	8.803 6.553	46.511 46.317	1.00 7.88	В
	ATOM	3517	C	LEU	132		43.882	8.393	46.295	1.00 13.99 1.00 14.28	B B
_	MOTA	3518	ŏ	LEU	132		43.737	8.410	47.526	1.00 13.98	В
45	ATOM	3519	N	ALA	133		42.947	8.832	45.443	1.00 13.83	В
	ATOM	3520	CA	ALA	. 133		41.651	9.342	45.909	1.00 12.82	B
	MOTA	3521	CB	ALA	133		40.796	9.805	44.733	1.00 12.54	В
	MOTA	3522	С	ALA	. 133		40.875	8.291	46.717	1.00 13.00	В
50	MOTA	3523	0	ALA	133		40.840	7.092	46.371	1.00 14.00	В
30	ATOM	3524	N	GLY	134		40.226	8.760	47.780	1.00 13.17	В
	MOTA	3525	CA	GLY	134		39.470	7.884	48.653	1.00 10.45	В
	MOTA MOTA	3526 3527	0	GLY	134 134	٠.	37.996	7.819 8.422	48.324	1.00 9.48	. в
	MOTA	3528	N	ILE	135		37.546 37.254	7.094	47.385 49.158	1.00 8.50	В
55	ATOM	3529	CA	ILE	135		35.820	6.874	48.981	1.00 10.67 1.00 9.46	B B
	ATOM	3530	CB	ILE	135		35.237	6.087	50.180	1.00 9.70	В
	MOTA	3531		ILE	135		33.709	5.990	50.079	1.00 10.21	В
	MOTA	3532	CG1	ILE	135		35.837	4.686	50.214	1.00 8.19	В.
~	MOTA	3533	CD1	ILE	135		35.426	3.864	51.452	1.00 8.61	В
60 ·	ATOM	3534	С	ILE	135		34.968	8.115	48.739	1.00 9.92	В
	MOTA	3535	0	ILE	135		34.135	8.150	47.812	1.00 7.51	В
	MOTA	3536	N	ILE	136		35.157	9.136	49.560	1.00 9.63	В
	MOTA	-3537	CA	ILE	136		34.379	10.340	.49.371	1.00 8.14	В
65	ATOM	3538	CB	ILE	136		34.671	11.371	50.500	1.00 6.28	В
UJ	MOTA	3539	CG2		136		33.997	12.691	50.166	1.00 6.74	В
	ATOM	3540	CG1		136		34.125	10.825	51.831	1.00 5.22	В
	MOTA MOTA	3541 3542	CD1 C	ILE	136		34.553	11.574	53.070	1.00 1.00	В
	MOTA	3542	0	ILE	136 136		34.538 33.569	10.992 11.242	47.978 47.274	1.00 9.33 1.00 10.23	В
70	ATOM	3544	N	PRO	137		35.767	11.252	47.552	1.00 10.23	B B
-	MOTA	3545	CD	PRO	137		37.096	11.215	48.163	1.00 7.00	B
	ATOM	3546	CA	PRO	137		35.816	11.874	46.234	1.00 7.00	В.
	MOTA	3547	CB	PRO	137		37.243	12.398	46.174	1.00 5.68	В

	MOTA	3548	CG	PRO	137	37.968	11.448	46.976	1.00 7.36	В
	MOTA	3549	С	PRO	137	35.370	10.967	45.098	1.00 7.27	В
	ATOM	3550	o'	PRO	137	34.857	11.434	44.120	1.00 9.92	B
_	MOTA	3551	N	ARG	138	35.547	9.661	45.233	1.00 7.38	В
5	ATOM	3552	CA	ARG	138	35.132	8.765	44.157	1.00 4.69	В
	ATOM .	3553	CB	ARG	138	35.761	7.375	44.314	1.00 5.18	В
	MOTA	3554	CG	ARG	138	37.257	7.373	44.145	1.00 4.97	В
	MOTA	3555	CD	ARG	138	37.858	6.057	44.522	1.00 8.61	В
••	ATOM	3556	NE	ARG	138	39.307	6.094	44.387	1.00 9.73	В
10	ATOM	3557	CZ	ARG	138	39.954	5.973	43.235	1.00 12.02	В
	MOTA	3558	NH1	ARG	138 .	39.279	5.799	42.102	1.00 12.04	. В
	MOTA	3559	NH2	ARG	138	41.280	6.028	43.216	1.00 13.69	В
	MOTA	3560	С	ARG	138	33.623	8.667	44.131	1.00 4.18	В
. ~	MOTA	3561	0	ARG	138	33.017	8.611	43.094	1.00 7.46	В
15	MOTA	3562	N	THR	139	33.013	8.666	45.295	1.00 3.72	В
	MOTA	3563	CA	THR	139	31.578	8.581	45.339	1.00 3.48	В
	MOTA	3564	CB	THR	139	31.103	8.436	46.792	1.00 2.17	В
	MOTA	3565		THR	139	31.647	7.220	47.321	1.00 4.08	В
20	MOTA	3566	CG2	THR	139	29.586	8.366	46.872	1.00 1.00	В
20	ATOM	3567	C	THR	139	30.956	9.798	44.677	1.00 4.20	В
	ATOM	3568	0	THR	139	30.178	9.666	43.727	1.00 5.38	В
	ATOM	3569	N	LEU	140	31.313	10.983	45.148	1.00 4.85	В
	MOTA	3570	CA	LEU	140	30.740	12.187	44.582	1.00 5.86	В
25	MOTA	3571	CB	LEU	140	31.374	13.423	45.207	1.00 4.02	В
23	ATOM	3572	CG	LEU	140	30.995	13.484	46.692	1.00 4.42	. B
	ATOM	3573		LEU	140	31.695	14.631	47.363	1.00 6.86	• В
	MOTA	3574		LEU	140	29.511	13.617	46.827	1.00 2.19	В
	MOTA	3575	C	LEU	140	30.902	12.211	43.091	1.00 8.32	В
30	MOTA	3576	0	LEU	140	29.958	12.523	42.378	1.00 10.70	В
50	ATOM	3577 3578	N	HIS	141	32.085	11.853	42.611	1.00 9.41	В
	MOTA MOTA	3579	CA CB	HIS	141	32.315	11.876 11.465	41.180 40.836	1.00 11.42	В
	ATOM	3580	CG	HIS	141 141	33.753 34.064	11.523	39.364		В
	MOTA	3581		HIS	141	34.074	10.555	38.413	1.00 15.31	B B
35	MOTA	3582		HIS	141	34.404	12.693	38.713	1.00 17.05	В
J	MOTA	3583		HIS	141	34.612	12.445	37.432	1.00 17.05	В
	ATOM	3584		HIS	141	34.418	11.154	37.225	1.00 15.55	В
	ATOM	3585	C	HIS	141	31.362	10.910	40.495	1.00 11.46	В
	ATOM	3586	ŏ	HIS	141	30.727	11.239	39.499	1.00 12.67	В
40	ATOM	3587	N	GLN	142	31.251	9.714	41.054	1.00 12.56	B
	ATOM	3588	CA	GLN	142	30.405	8.694	40.464	1.00 12.86	В
	ATOM	3589	CB	GLN	142	30.707	7.336	41.103	1.00 14.29	В
	ATOM	3590	CG	GLN	142	32.000	6.739	40.590	1.00 18.45	В
	ATOM	3591	CD	GLN	142	32.012	6.628	39.068	1.00 21.75	В
45	MOTA	3592		GLN	142	31.349	5.751	38.489	1.00 23.11	В
	ATOM	3593		GLN	142	32.743	7.535	38.408	1.00 20.86	В
	MOTA	3594	С	GLN	142	28.915	B.984	40.473	1.00 12.11	В
	MOTA	3595	0	GLN	142	28.206	8.585	39.560	1.00 11.87	В
	MOTA	3596	N	ILE	143	28.434	9.664	41.506	1.00 11.12	В
50	MOTA	3597	CA	ILE	143	27.018	10.010	41.573	1.00 12.39	В
	MOTA	3598	CB	ILE	143	26.722	10.953	42.788	1.00 12.55	В
	ATOM	3599	CG2	ILE	143	25.341	11.608	42.650	1.00 12.75	В
	ATOM	3600	CG1	ILE	143	26.784	10.147	44.093	1.00 13.10	В
E E	MOTA	3601		ILE	143	26.532	10.971	45.338	1.00 10.72	В
55	MOTA	3602	С	ILE	143	26.587	10.710	40.275	1.00 13.82	В
	MOTA	3603	0	ILE	143	25.541	10.391	39.705	1.00 14.18	В
	MOTA	3604	N	PHE	144	27.397	11.666	39.816	1.00 14.48	В
	MOTA	3605	CA	PHE	144	27.099	12.430	38.605	1.00 15.02	В
60	MOTA	3606	CB	PHE	144	28.023	13.646	38.513	1.00 14.03	В
60	ATOM	3607	CG	PHE	144	27.773	14.676	39.585	1.00 12.67	В
	MOTA	3608		PHE	144	26.680	15.527	39.510	1.00 10.36	В
	ATOM	3609	CD2		144	28.623	14.796	40.678	1.00 13.84	В
	MOTA	3610	CE1		144	26.442	16.473	40.498	1.00 9.69	В.
65	ATOM	3611	CE2		144	28.375	15.761	41.680	1.00 13.70	В
UJ.	ATOM	3612	cz	PHE	144	27.286	16.591	41.578	1.00 11.21	В
	ATOM	3613	C	PHE	144	27.223	11.586	37.348	1.00 16.57	В
	ATOM	3614	0	PHE	144	26.516	11.835	36.384	1.00 16.66	В
	ATOM	3615	N	GLU	145	28.123	10.593	37.364	1.00 20.10	В
70	ATOM	3616	CA	GLU	145	28.335	9.691	36.210	1.00 22.03	В
10	MOTA	3617 3618	CB	GLU	145	29.597	8.825	36.352	1.00 26.12	В
	MOTA MOTA	3618	CG	GLU	145	30.902	9.538	36.044	1.00 32.68	В
	MOTA	3620	CD	GLU	145	31.004	9.949	34.595 34.249	1.00 36.87	В
	ALUM	3020	OEI	GDU	145	31.965	10.666	34.249	1.00 39.57	В

•	MOTA	3621	OE2	GLU	145	30.121	9.549	33.807	1.00 40.00	В
	MOTA	3622	С	GLU	145	27.194	8.705	36.029	1.00 21.04	В
	ATOM	3623	ō	GLU	145	26.750	8.470	34.943	1.00 20.94	В
	ATOM	3624	N	LYS	146	26.728	8.129	37.127	1.00 22.01	В
5										
J	ATOM	3625	CA	LYS	146	25.628	7.166	37.072	1.00 22.94	В
	MOTA	3626	CB	LYS	146	25.489	6.433	38.423	1.00 24.69	В
	ATOM	3627	CG	LYS	146 .	26.725	5.599	38.799	1.00 27.30	В
	MOTA	3628	CD	LYS	146	26.480	4.519	39.854	1.00 24.53	В
	MOTA	3629	CE	LYS	146	27.560	3.447	39.715	1.00 25.61	В
10	ATOM	3630	NZ	LYS	146	27.404	2.262	40.595	1.00 24.71	В
10					146	24.281	7.799	36.702	1.00 24.71	В
	ATOM	3631	C	LYS						
	ATOM	3632	0	LYS	146	23.472	7.178	36.020	1.00 24.07	В
	ATOM	3633	N	LEU	147 .	24.049	9.035	37.138	1.00 23.75	В
	MOTA	3634	CA	LEU	147	22.788	9.720	36, 850	1.00 24.08	В
15	MOTA	3635	CB	LEU	147	22.247	10.365	38.123	1.00 24.33	В
	ATOM	3636	CG	LEU	147	21.976	9.460	39.325	1.00 24.88	В
•	ATOM	3637		LEU	147	21.607	10.299	40.537	1.00 24.59	B
	MOTA	3638		LEU	147	20.847	8.493	39.014	1.00 24.04	В
20	ATOM	3639	С	LEU	147 .	22.895	10.796	35.762	1.00 25.02	В
20	ATOM	3640	0	LEU	147	22.110	11.755	35.736	1.00 22.56	В
	ATOM	3641	N	THR	148	23.857	10.627	34.857	1.00 27.04	В
	ATOM	3642	CA	THR	148	24.073	11.585	33.774	1.00 28.40	В.
	MOTA	3643	СВ	THR	148	25.296	11.194	32.905	1.00 28.80	В.
25	MOTA	3644		THR	148	25.479	12.150	31.850	1.00 29.27	. B
23	MOTA	3645	CG2	THR	148	25.108	9.794	32.318	1.00 30.26	В
	MOTA	3646	C	THR	148	22.855	11.738	32.865	1.00 28.70	В
	ATOM	3647	0	THR	148	22.466	12.848	32.580	1.00 29.54	В
	ATOM	3648	N	ASP	149	22.253	10.638	32.413	1.00 27.95	В
	ATOM	3649	CA	ASP	149	21.087	10.749	31.533	1.00 28.50	В
30	MOTA	3650	CB	ASP	149	21.500	11.014	30.067	1.00 28.76	В
50										
	MOTA	3651	CG	ASP	149	22.520	10.010	29.522	1.00 29.99	В
	MOTA	3652		ASP	149	22.501	8.830	29.939	1.00 29.75	В
	MOTA	3653	OD2	ASP	149	23.332	10.408	28.646	1.00 29.41	В
	MOTA	3654	С	ASP	149	20.148	9.551	31.576	1.00 28.84	В
35	MOTA	3655	0	ASP	149	19.636	9.096	30.555	1.00 27.84	В
	MOTA	3656	N	ASN	150	19.899	9.055	32.778	1.00 29.57	В
	MOTA	3657	CA	ASN	150	19.008	7.912	32.928	1.00 31.21	В
	ATOM	3658	СВ	ASN	150	19.483	7.010	34.080	1.00 29.55	В
40	MOTA	3659	CG	ASN	150	19.259	7.641	35.459	1.00 28.21	В
40	MOTA	3660	OD1	asn	150	19.347	8.859	35.618	1.00 27.26	В
	MOTA	3661	ND2	ASN	150	18.969	6.804	36.458	1.00 25.05	В
	MOTA	3662	С	ASN	150	17.550	8.345	33.175	1.00 31.80	В
	ATOM	3663	ŏ	ASN	150	16.693	7.501	33.485	1.00 32.95	В
	ATOM	3664		GLY	151	17.279	9.648	33.043		
45		_	N						1.00 30.56	В
43	MOTA	3665	CA	GLY	151	15.939	10.169	33.247	1.00 29.70	B
	ATOM	3666	С	GLY	151	15.601	10.387	34.701	1.00 29.38	В
	MOTA	3667	0 -	GLY	151	14.462	10.518	35.052	1.00 29.95	В
	MOTA	3668	N	THR	. 152	16.616	10.412	35.549	1.00 29.90	В
	MOTA	3669	CA'	THR	152	16.386	10.634	36.964	1.00 30.17	В
50	ATOM	3670	CB	THR	152	17.082	9.552	37.805	1.00 29.93	В
50	ATOM	3671	OG1	THR	152					
						16.662	8.249	37.373	1.00 29.92	В
	MOTA	3672	CG2		152	16.739	9.730	39.272	1.00 31.14	В
	MOTA	3673	С	THR	152	16.902	12.022	37.384	1.00 31.11	В
	ATOM	3674	0	THR	152	18.104	12.232	37.543	1.00 32.13	В
55	MOTA	3675	N	GLU	153	15.977	12.968	37.531	1.00 30.29	В
	ATOM	3676	CA	GLU	153	16.310	14.325	37.948	1.00 28.58	В
	ATOM	3677	СВ	GLU	153	15.041	15.174	37.977	1.00 31.74	В
						15.041				_
	ATOM	3678	CG	GLU	153	15.257	16.669	37.853	1.00 35.57	₿.
60	MOTA	3679	CD	GLU	153	15.641	17.082	36.438	1.00 38.01	В
60	MOTA	3680	OE1	GLU	153	15.923	18.281	36.200	1.00 38.59	В
	MOTA	3681	OE2	GLU	153	15.655	16.201	35.551	1.00 39.17	В
	MOTA	3682	C	GLU	153	16.861	14.173	39.366	1.00 25.90	В
	ATOM	3683	ō	GLU	153	16.382	13.346	40.114	1.00 25.18	В
	ATOM	3684	Ň	PHE	154	17.852	14.978	39.738	1.00 24.45	
65										В
U)	MOTA	3685	CA	PHE	154	18.447	14.852	41.074	1.00 21.39	В
	MOTA	3686	CB	PHE	154	19.411	13.651	41.115	1.00 20.65	В
	MOTA	3687	CG	PHE	154	20.679	13.846	40.306	1.00 20.31	В
	ATOM	3688	CD1	PHE	154	21.853	14.284	40.904	1.00 19.86	В
	ATOM	3689		PHE	1.54	20.698	13.570	38.945	1.00 19.64	В
70	ATOM	3690		PHE	154	23.021	14.435	40.142	1.00 21.56	B
. •	ATOM	3691		PHE	154	21.856	13.720	38.194	1.00 20.70	. В
	ATOM	3692	CZ.	PHE	154	23.017	14.149	38.786	1.00 19.85	В
	MOTA	3693	С	PHE	154	19.224	16.073	41.567	1.00 19.03	В

	ATOM	3694	0	PHE	154	19.579	16.970	40.805	1.00 18.07	В
	ATOM	3695	N	SER	155	19.470	16.107	42.865	1.00 17.25	В
	ATOM	3696	ĊA	SER	155	20.234	17.200	43.451	1.00 17.56	В
_	MOTA	3697	СВ	SER	155	19.310	18.302	44.043	1.00 18.40	В
5	MOTA	3698	OG	SER	155	. 18.744	17.999	45.315	1.00 19.07	В
	MOTA	3699	C	SER	155	21.072	16.536	44.521	1.00 16.97	В
	ATOM	3700	ŏ	SER	155	20.629	15.587	45.157	1.00 15.32	В
	MOTA	3701	N	VAL	156	22.286	17.034	44.708	1.00 17.21	В
	MOTA	3702	CA	VAL	156	23.181 -	16.479	45.709	1.00 15.73	В
10	ATOM	3703	CB	VAL	156	24.452	15.964	45.066	1.00 16.35	В
	MOTA	3704	CG1	VAL	156	25.307	15.319	46.089	1.00 16.70	• В
	MOTA	3705			156	24.117	14.993	43.973	1.00 18.36	. в
	MOTA	3706	С	VAL	156	23.577	17.503	46.762	1.00 14.63	В
	MOTA	3707	0	VAL	156	24.031	18.595	46.441	1.00 12.84	В
15	MOTA	3708	N	LYS	157	23.394	17.138	48.024	1.00 15.08	В
	ATOM	3709	CA.	LYS	157	23.739	18.019	49.139	1.00 16.33	В
	MOTA	3710	CB	LYS	157	22.485	18.370	49.962	1.00 17.27	В
	ATOM	3711	CC	LY\$	157	21.640	19.492	49.381	1.00 19.38	В
	MOTA	3712	CD	LYS	157	20.323	19.704	50.121	1.00 19.23	В
20	ATOM	3713	CE	LYS	157 ·	19.563	20.911	49.535	1.00 20.48	В
	ATOM	3714	NZ	LYS	157	20.216	22.239	49.815	1.00 19.89	В
					157					
	MOTA	3715	C	LYS		24.738	17.288	50.025	1.00 15.63	В
	MOTA	3716	0	LYS	157	24.568	16.118	50.305	1.00 17.71	В
~-	MOTA	3717	N	VAL	158	25.789	17.979	50.447	1.00 14.09	В
25	MOTA	3718	CA	VAL	158	26.782	17.350	51.313	1.00 12.31	• В
	ATOM	3719	СВ	VAL	158	28.184	17.314	50.670	1.00 11.69	. В
								49.405	1.00 12.25	
	MOTA	3720		·VAL	158	28.150	16.490			В
	MOTA	3721	CG2	VAL	158	28.657	18.731	50.367	1.00 11.55	В
	MOTA	3722	С	VAL	158	26.911	18.070	52.636	1.00 11.94	В
30	MOTA	3723	0	VAL	158	26.668	19.270	52.726	1.00 11.97	В
	ATOM	3724	N	SER	159	27.301	17.321	53.659	1.00 10.91	В
	ATOM	3725	CA	SER	159	27.490	17.876	54.992	1.00 11.22	В
	MOTA	3726	СВ	SER	159	26.245	17.662	55.B46	1.00 11.02	В
	ATOM	3727	OG	SER	159	25.184	18.476	55.385	1.00 17.68	В
35	MOTA	3728	С	SER	159	28.677	17.212	55.667	1.00 11.18	В
	MOTA	3729	ō	SER	159	28.925	16.002	55.499	1.00 10.26	. В
	MOTA	3730	N	LEU	160	29.431	18.011	56.405	1.00 11.19	В
	MOTA	3731	ÇA	LEU	. 160	30.583	17.495	57.115	1.00 11.64	В
: -	ATOM	3732	CB	LEU	160	31.875	18.043	56.498	1.00 11.99	В
40	MOTA	3733	CG	LEU	160	33.168	17.440	57.061	1.00 12.29	B
. •	ATOM	3734		LEU	160	33.088	15.915	57.170	1.00 12.16	В
	MOTA	3735	CD2	LEU	160	34.307	17.848	56.170	1.00 13.02	В
	MOTA	3736	С	LEU	160	30.476	17.836	58.606	1.00 12.31	В
	ATOM	3737	0	LEU	160	30.894	18.913	59.056	1.00 13.72	В
45	MOTA	3738	N	LEU	161	29.921	16.899	59.365	1.00 11.68	В
	MOTA	3739	CA	LEU	161	29.728	17.056	60.794	1.00 11.73	В
	MOTA	3740	CB	LEU	161	28.387	16.462	61.184	1.00 10.86	В
	MOTA	3741	CG	LEU	161	28.069	16.373	62.667	1.00 11.21	В
	ATOM	3742	CD1	LEU	161	28.038	17.772	63.257	1.00 14.64	В
50	ATOM	3743	CD2	LEU	161	26.735	15.687	62.849	1.00 11:87	В
	ATOM	3744	С	LEU	161	30.805	16.318	61.565	1.00 11.76	В
	MOTA	3745	ŏ	LEU		31.023	15.148	61.353		
					161				1.00 14.92	В
	MOTA	3746	N	GLU	162	31.493	17.005	62.461	1.00 11.26	В
	MOTA	3747	CA	GLU	162	32.536	16.335	63.230	1.00 10.12	В
55	MOTA	374B	CB	GLU	162	33.914	16.845	62.829	1.00 9.47	В
	ATOM	3749	CG	GLU	162	34.143	16.845	61.353	1.00 9.35	В
	ATOM	3750	ÇD	GLU	162	35.607	16.813	61.008		B
	ATOM	3751		GLU	162	36.443	17.239	61.829	1.00 9.19	В
60	MOTA	3752		GLU	162	35.929	16.357	59.901	1.00 8.99	В
60	ATOM	3753	С	GLU	162	32.339	16.498	64.729	1.00 10.38	В
	ATOM	3754	0	GLU	162	31.849	17.527	65.222	1.00 7.96	В
	ATOM	3755	N	ILE	163	32.734	15.456	65.444	1.00 10.66	В
	ATOM	3756	CA	ILE	163	32.581	15.414	66.879	1.00 10.98	В.
65	MOTA	3757	СВ	ILE	163	31.782	14.160	67.293	1.00 11.27	В
65	ATOM	3758	CG2	ILE	163	31.505	14.192	68.793	1.00 11.05	В
	ATOM	3759		ILE	163	30.504	14.066	66.462	1.00 11.37	В
	ATOM	3760		ILE	163	29.804	12.728	66.528	1.00 12.73	
										В
	MOTA	3761	C	ILE	163	33.941	15.387	67.559	1.00 10.94	В
70	MOTA	3762	0	ILE	163	34.849	14.680	67.127	1.00 11.24	В
70	MOTA	3763	N	TYR	164	34.071	16.177	68.619	1.00 10.16	В
	MOTA	3764	CA	TYR	164	35.303	16.245	69.376	1.00 8.14	В
	ATOM	3765	СВ	TYR	164	36.254	17.270	68.759	1.00 5.82	В
	ATOM	3766	CG	TYR	164	37.517	17.425	69.533	1.00 3.86	В

•	MOTA	3767	CD1	TYR	164	37.560	18.215	70.682	1.00 5.62	В
	ATOM	3768	CE1		164	38.709	18.292	71.465	1.00 4.56	В
	ATOM	3769	CD2	TYR	164	38.651	16.719	69.177	1.00 3.71	. В
5	MOTA	3770	CE2	TYR	164	39.811	16.786	69.955		В
5	ATOM	3771	CZ	TYR	164	39.827	17.577	71.094	1.00 4.77	В
	ATOM	3772	OH	TYR	164	40.976	17.675	71.832	1.00 5.42	В
	ATOM '	3773	С	TYR	164	34.937	16.617	70.802	1.00 8.94	В
	ATOM	3774	ō	TYR	164	34.299	17.627	71.061	1.00 9.91	В
		3775			165	35.346	15.775	71.731	1.00 10.87	В
10	ATOM		N	ASN						
10	MOTA	3776	CA	ASN	165	35.050	16.003	73.134	1.00 12.54	₿
	MOTA	3777	CB	ASN	165	35.847	17.192	73.674	1.00 15.11	В
	ATOM	3778	CG	ASN	165	35.722	17.336	75.190	1.00 19.28	В
	MOTA	3779	OD1	ASN	165 .	35.971	16.385	75.936	1.00 21.80	В
•	ATOM	3780		ASN	165	35.345	18.528	75.651	1.00 20.20	В
15										
13	ATOM	3781	С	ASN	165	33.562	16.262	73.308	1.00 12.20	В
	MOTA	3782	0	ASN	165	33.160	17.158	74.000	1.00 10.80	В
	ATOM	3783	N	GLU	166	32.767	15.430	72.646	1.00 16.33	В
	ATOM	3784	CA	GLU	166	31.304	15.495	72.656	1.00 18.28	В
	ATOM	3785	CB	GLU	166	30.739	15.101	74.031	1.00 17.10	В
20	ATOM	3786	CG	GLU	166	30.887	13.610	74.353	1.00 16.82	В
20										
	MOTA	3787	CD	GLU	166	30.175	12.693	73.357	1.00 16.06	В
	MOTA	3788	OE1	GLU	166	28.928	12.606	73.360	1.00 13.96	В.
	MOTA	3789	OE2	GLU	166	30.880	12.055	72.559	1.00 15.35	В
	MOTA	3790	C	GLU	166	30.697	16.825	72.201	1.00 19.60	• В
25	ATOM	3791	ō	GLU	166	29.604	17.192	72.606	1.00 19.36	В
						31.427		71.357	1.00 21.89	
	MOTA	3792	N	GLU	167		17.546			В
	MOTA	3793	CA	GLU	167	30.956	18.818	70.823	1.00 22.41	В
	MOTA	3794	СВ	GLU	167	31.910	19.947	71.208	1.00 24.57	В
	MOTA	3795	CG	GLU	167	31.998	20.181	72.701	1.00 28.83	· в
30	MOTA	3796	CD	GLU	167	32.847	21.376	73.044	1.00 31.70	В
• •	ATOM	3797		GLU	167	33.985	21.472	72.521	1.00 32.58	В
	MOTA	3798	OE2	GLU	167	32.373	22.214	73.840	1.00 33.47	В
	MOTA	3799	·C	GLU	167	30.874	18.683	69.314	1.00 21.24	В
	MOTA	3800	0	GLU	167	31.689	17.997	68.700	1.00 20.64	В
35	MOTA	·3801	N	LEU	168	29.879	19.328	68.717	1.00 20.17	В
	MOTA	3802	CA	LEU	168	29.712	19.254	67.269	1.00 19.71	В
	ATOM	3803	CB	LEU	168	28.240	19.110	66.887	1.00 19.82	В
	MOTA	3804	CG	LEU		27.430		67.457	1.00 19.46	В
40	MOTA	3805		LEU	168	28.198	16.653	67.320	1.00 19.39	В
40	MOTA	3806	CD2	LEU	168	27.113	18.236	68.903	1.00 20.70	В
	MOTA	3807	С	LEU	168	30.251	20.477	66.524	1.00 19.80	В
	MOTA.	3808	0	LEU	168	30.055	21.611	66.939	1.00 20.40	В
	ATOM	3809	Ń	PHE	169	30.928	20.229	65.411	1.00 19.38	В
45	MOTA	3810	CA	PHE	169	31.478	21.306	64.612	1.00 17.82	В
43	MOTA	3811	CB	PHE	169	33.004	21.327	64.706	1.00 17.88	В
	ATOM	3812	CG	PHE	169	33.513	21.530	66.097	1.00 16.09	В
	MOTA	3813	CD1	PHE	169	33.737	20.445	66.928	1.00 15.76	В
	ATOM	3814	CD2	PHE	. 169	33.695	22.810	66.600	1.00 16.92	В
	ATOM	3815		PHE	169	34.130	20.621	68.235	1.00 16.10	В
50	ATOM	3816		PHE	169	34.090	23.001	67.907	1.00 17.09	В
, 50										
	MOTA	3817	CZ	PHE	169	34.308	21.901	68.731	1.00 16.73	В
	ATOM	3818	С	PHE	169	31.068	21.102	63.166	1.00 18.77	. В
	MOTA	3819	0	PHE	169	30.929	19.980	62.704	1.00 18.62	В
	ATOM	3820	N	ASP	170	30.871	22.206	62.459	1.00 20.24	В
55	MOTA	3821	CA	ASP	170	30.476	22.171	61.055	1.00 21.83	В
	MOTA	3822	СВ	ASP	170	29.387	23.216	60.785	1.00 20.71	В
	MOTA		CG						1.00 22.77	В
		3823		ASP	170	28.832	23.135	59.382		
	MOTA	3824		ASP	170	29.510	22.563	58.493	1.00 23.50	₿.
	MOTA	3825	OD2	ASP	170	27.724	23.658	59.158	1.00 24.44	В
60	MOTA	3826	C .	ASP	170	31.714	22.545	60.269	1.00 22.03	В
	MOTA	3827	0	ASP	170	32.119	23.693	60.281	1.00 23.16	В
	MOTA	3828	N	LEU	171	32.320	21.577	59.593	1.00 21.95	В
					171	33.514				
	ATOM	3829	CA	LEU			21.878	.58.828	1.00 22.12	В
65	MOTA	3830	CB	LEU	171	34.449	20.674	58.827	1.00 20.38	В
65	MOTA	3831	CG	LEU	171	35.422	20.605	60.013	1.00 21.16	₿.
	MOTA	3832		LEU	171	36.359	21.824	60.018	1.00 20.44	В
	MOTA	3833		LEU	171	34.645	20.544	61.307	1.00 18.78	В
	MOTA	3834	Ċ	LEU	171	33.271	22.356	57.402	1.00 24.20	В
	ATOM	3835	ŏ	LEU	171	34.201	22.357	56.582	1.00 24.74	В
70					172					
70	ATOM	3836	N	LEU		32.034	22.764	57.108	1.00 26.40	В
	MOTA	3837	CA	LEU	172	31.686	23.266	55.776	1.00 28.39	В
	MOTA	3838	CB	LEŲ	172	30.802	22.283	55.004	1.00 28.49	В
	MOTA	3839	CG	LEU	172	31.536	21.056	54.448	1.00 29.54	В

	ATOM	3840	CD1	LEU	172	30.562	20.216	53.633	1.00 30.71	В
	ATOM	3841		LEU	172	32.730	21.477	53.583	1.00 28.53	В
	ATOM	3842	C	LEU	172	30.979	24.607	55.797	1.00 28.89	В
	MOTA	3843	O	LEU	172	30.416	25.030	54.823	1.00 30.09	В
5	MOTA	3844	N	ASN	173	31.007	25.264	56.941	1.00 31.10	В
	ATOM .		CA	ASN	173	30.403	26.580	57.043	1.00 34.00	. в
	MOTA	3846	CB	ASN	173	29.606	26.708	58.347	1.00 33.23	В
	ATOM	3847	CG	ASN	173	28.903	28.053	58.473	1.00 32.72	В
. 2	ATOM	3848	OD1	ASN	173	28.108	28.268	59.381	1.00 33.30	В
10	ATOM	3849	ND2	ASN	173	29.205	28.967	57.551	1.00 31.17	В
	MOTA	3850	С	ASN	173	31.554	27.579	56.982	1.00 35.93	· В
	ATOM	3851	0	ASN	173	32.402	27.627	57.861	1.00 35.47	В
	ATOM	3852	N	PRO	174	31.609	28.372	55.908	1.00 38.25	В
'	MOTA	3853	CD	PRO	174	30.799	28.283	54.681	1.00 38.57	В
15	MOTA	3854	CA	PRO	174	32.674	29.362	55.753	1.00 40.38	В
	MOTA	3855	CB	PRO	174	32.702	29.569	54.242	1.00 39.65	В
	MOTA	3856	CG	PRO	174	31.264	29.478	53.900	1.00 38.79	В
	MOTA	3857	С	PRO	174	32.445	30.632	56.582	1.00 42.95	В
00	MOTA	3858	0	PRO	174	33.356	31.450	56.743	1.00 43.55	В
20	MOTA	3859	N	SER	175	31.234	30.794	57.108	1.00 45.10	В
	MOTA	3860	CA	SER	175	30.906	31.974	57.913	1.00 47.15	В
	MOTA	3861	CB	SER	175	29.395	32.227	57.889	1.00 47.30	В
	MOTA	3862	0G	SER	175	28.906	32.331	56.559	1.00 49.37	В
25	MOTA	3863	C	SER	175	31.369	31.882.	59.376	1.00 47.57	В
25	ATOM	3864	0	SER	175	31.800	32.872	59.970	1.00 48.25	В
	ATOM	3865	N	SER	176	31.280	30.690	59.953	1.00 47.97	· B
	MOTA	3866	CA	SER	176	31.677	30.487	61.340	1.00 47.64	В
	MOTA	3867	CB	SER	176	30.720	29.520	62.034	1.00 46.90	В
30	MOTA	3868	OG O	SER	176	30.794	28.230	61.447	1.00 46.36	В
50	ATOM	3869	c	SER	176	33.083	29.917	61.451	1.00 48.54	В
	MOTA	3870	0	SER	176	33.650 33.646	29.434	60.484 62.648	1.00 48.78	В
	MOTA MOTA	3871 3872	N CA	ASP ASP	177 177		29.989 29.467		1.00 49.43 1.00 50.07	В
	MOTA	3873	CB	ASP	177	34.979 35.843	30.521	62.874		В
35	ATOM	3874	CG	ASP	177	35.342	30.852	63.591 64.996	1.00 51.58	В
22	ATOM	3875		ASP	177	35.948	31.723	65.658	1.00 53.37	B B
	MOTA	3876		ASP	177	34.353	30.246	65.452	1.00 54.61	В
	ATOM	3877	C	ASP	177	34.880	28.160	63.669	1.00 49.81	В
	ATOM	3878	ŏ	ASP	177	33.833	27.830	64.235	1.00 48.89	В
40	ATOM	3879	N	VAL	178	35.980	27.422	63.707	1.00 49.42	В
	ATOM	3880	CA	VAL	178	36.030	26.146	64.409	1.00 50.03	В
	ATOM	3881	СВ	VAL	178	37.385	25.452	64.150	1.00 50.76	В
	ATOM	3882		VAL	178	37.528	25.131	62.665	1.00 49.77	В
	ATOM	3883		VAL	178	38.538	26.353	64.629	1.00 50.93	B
45	MOTA	3884	c	VAL	178	35.791	26.203	65.927	1.00 49.82	В
	ATOM	3885	ŏ	VAL	178	35.912	25.194	66.623	1.00 50.17	В
	ATOM	3886	N	SER	179	35.451	27.372	66.447	1.00 48.85	В
	ATOM	3887	CA	SER	179	35.225	27.491	67.877	1.00 47.91	В
	MOTA	3888	CB	SER	179	35.912	28.749	68.397	1.00 48.14	В
50	MOTA	3889	OG	SER	179	35.472	29.884	67.667	1.00 47.90	В
	MOTA	3890	С	SER	179	33.739	27.541	68.211	1.00 47.46	В
	MOTA	3891	0	SER	179	33.357	27.618	69.376	1.00 47.10	В
	MOTA	3892	N	GLU	180	32.900	27.495	67.182	1.00 46.50	В
	MOTA	3893	CA	GLU	180	31.458	27.542	67.383	1.00 45.18	В
55	MOTA	3894	CB	GLU	180	30.835	28.527	66.383	1.00 44.47	В
	MOTA	3895	CG	GLU	180	31.026	29.983	66.788	1.00 44.05	В
	ATOM	3896	CD	GLU	180		30.971	65.724	1.00 43.63	В
	MOTA	3897		GLU	180	31.354	31.176	64.751	1.00 43.67	В
۲۸	MOTA	3898		GLU	180	29.495	31.542	65.860	1.00 42.55	В
60	MOTA	3899	С	GLU	180	30.813	26.156	67.295	1.00 44.60	В
	ATOM	3900	0	GLU	180	30.714	25.570	66.228	1.00 44.37	В
	MOTA	3901	N	ARG	181	30.373	25.650	68.445	1.00 44.01	В
	MOTA	3902	CA	ARG	181	29.739	24.342	68.529	1.00 42.83	В
65	ATOM	3903	CB	ARG	181	29.775	23.806	69.958	1.00 45.18	В
65	MOTA	3904	CG	ARG	181	28.755	24.439	70.895	1.00 47.37	В
	MOTA	3905	CD	ARG	181	28.693	23.644	72.187	1.00 51.45	В
	MOTA	3906	NE	ARG	181	27.541	23.972	73.034	1.00 54.79	В
	MOTA	3907	CZ	ARG	181	26.267	23.753	72.706	1.00 56.32	В
70	ATOM	3908	NH1		181	25.969	23.205	71.539	1.00 57.53	В
10	ATOM	3909	NH2		181	25.286	24.065	73.548	1.00 56.18	В
	MOTA	3910	C	ARG	181	28.278	24.404	68.121	1.00 40.59	В
	MOTA	3911	O N	ARG	181	27.632	25.414	68.254	1.00 41.20	В
	MOTA	3912	14	LEU	182	27.759	23.293	67.632	1.00 38.61	В

•	ATOM	3913	CA	LEU	182	26.370	23:253	67.219	1.00 35.94	В
	MOTA	3914	CB	LEU	182	26.259	22.490	65.897	1.00 34.47	В
	ATOM	3915	CG	LEU	182	27.018	23.098	64.718	1.00 31.55	B
	ATOM	3916		LEU	182	26.951	22.179	63.525	1.00 30.32	B
5										
,	ATOM	3917		LEU	182	26.417	24.440	64.382	1.00 29.89	В
	ATOM	3918	С	LEU	182	25.532	22.579	68.300		В
	MOTA	3919	0	LEU	182	26.057	21.845	69.139	1.00 35.35	B
•	ATOM	3920	N	GLN	183	24.227	22.839	68.270	1.00 35.14	В
	MOTA	3921	CA	GLN	183	23.290	22.256	69.228	1.00 33.43	В
10	MOTA	3922	CB	GLN	183	22.261	23.284	69.688	1.00 36.19	В
	MOTA	3923	·CG	GLN	183	22.844	24.463	70.456	1.00 40.60	В
	ATOM	3924	CD	GLN	183	21.781	25.458	70.916	1.00 43.17	В
	MOTA	3925		GLN	183	20.902	25.122	71.711	1.00 45.10	В
• -	ATOM	3926	NE2	GLN	183	21.856	26.687	70, 408	1.00 42.17	В
15	ATOM	3927	С	GLN	183	22.513	21.122	68.578	1.00 30.84	В
	MOTA	3928	0	GLN	183	22.098	21.224	67.436	1.00 29.43	В
	MOTA	3929	N	MET	184	22.311	20.047	69.325	1.00 29.11	В
	ATOM	3930	CA	MET	184	21.603	18.884	68.821	1.00 28.51	В
	ATOM	3931		MET	184	22.549	17.698			
20			CB					68.930	1.00 27.68	В
20	MOTA	3932	CG	MET	184	21.997	16.385	68.443	1.00 30.34	В
	MOTA	3933	SD	MET	184	23.142	15.021	68.745	1.00 30.67	В
	ATOM	3934	CE	MET	184	22.841	14.793	70.448	1.00 30.06	В.
	ATOM	3935	C	MET	184	20.298	18.650	69.595	1.00 29.09	В
	ATOM	3936	0	MET	184	20.280	18.737	70.806	1.00 29.05	· B
25	ATOM	3937	N	PHE	185	19.213	18.342	68.887	1.00 30.68	В
	ATOM	3938	CA	PHE	185	17.921	18.112	69.537	1.00 31.83	В
	ATOM	3939	CB	PHE	185		19.277	69.291		
						16.953			1.00 31.45	В
	MOTA	3940	CG	PHE	185	17.520	20.626	69.637	1.00 30.24	В
20	MOTA	3941		PHE	185	18.381	21.275	68.763	1.00 29.12	В
30	MOTA	3942	CD2	PHE	185	17.215	21.234	70.850	1.00 28.98	В
	MOTA	3943	CE1	PHE	185	18.929	22.500	69.082	1.00 28.97	В
	ATOM	3944	CE2	PHE	185	17.762	22.461	71.180	1.00 29.87	В
•	MOTA	3945	CZ	PHE	185	18.624	23.098	70.289	1.00 29.79	В
	MOTA	3946	č	PHE	185	17.236	16.883	68.976	1.00 33.71	В
35	ATOM .	3947	ŏ		185					
55				PHE		17.473	16.515	67.845	1.00 33.43	В
	MOTA	3948	N	ASP	186	16.393	16.245	69.782	1.00 37.53	В
	MOTA	3949	CA	ASP	186	15.667	15.071	69.310	1.00 40.98	В
	ATOM	3950	CB	ASP	186	14.857	14.413	70.431	1.00 43.17	В
	ATOM	3951	CG	ASP	186	15.721	13.931	71.575	1.00 45.72	В
40	MOTA	3952	OD1	ASP	186	16.691	13.190	71.316	1.00 48.29	В
	ATOM	3953		ASP	186	15.413	14.291	72.734	1.00 46.64	В
	ATOM	3954	Ċ	ASP	186	14.676	15.587	68.284	1.00 42.58	В
	ATOM	3955		ASP	186	14.123				
			0				16.666	68.453	1.00 42.55	В
45	ATOM	3956	N	ASP	187	14.457	14.835	67.214	1.00 44.89	В
43	MOTA	3957	CA	ASP	187	13.528	15.287	66.188	1.00 46.96	В
	ATOM	3958	CB	ASP	187	13.921	14.695	64.840	1.00 46.66	В
	ATOM	3959	CG	ASP	187	13.090	15.232	63.718	1.00 46.68	В
	ATOM	3960	OD1	ASP	187	13.381	14.891	62.555	1.00 47.95	В
	MOTA	3961		ASP	187	12.144	15.996	64.008	1.00 45.37	B
50	ATOM	3962	C	ASP	187	12.127	14.881	66.604	1.00 48.78	В
-	MOTA	3963	ŏ	ASP	187		13.696			
						11.844		66.773	1.00 49.04	В
	MOTA	3964	N	PRO	188	11.235	15, 870	66.799	1.00 50.85	В
	MOTA	3965	CD	PRO	188	11.546	17.310	66.716	1.00 50.78	В
	ATOM	3966	CA	PRO	188	9.838	15.660	67.209	1.00 52.07	В
55	MOTA	3967	CB	PRO	188	9.280	17.085	67.240	1.00 51.41	В
	ATOM	3968	CG	PRO	188	10.496	17.916	67.605	1.00 50.84	В
	MOTA	3969	С	PRO	188	9.071	14.705	66.302	1.00 53.79	В
	ATOM	3970	ō	PRO	188	8.249	13.900	66.753	1.00 52.56	В.
	MOTA	3971	N	ARG	189	9.340	14.817	65.011	1.00 56.26	
60										В
oo	ATOM	3972	CA.	ARG	189	8.691	13.979	64.033	1.00 59.28	В
	MOTA	3973	CB	ARG	189	9.218	14.349	62.649	1.00 60.03	В
	MOTA	3974	CG	ARG	189	8.875	15.774	62.238	1.00 61.54	В
	MOTA	3975	CD	ARG	189	9.366	16.081	60.833	1.00 62.62	В
	ATOM	3976	NE	ARG	189	10.813	16.277	60.790	1.00 63.59	В
65	ATOM	3977	CZ	ARG	189	11.407	17.465	60.837	1.00 64.36	В
	ATOM	3978	NH1		189	10.680	18.575	60.925	1.00 64.67	В
		3979	NH2							
	MOTA				189	12.729	17.545	60.794	1.00 64.73	В
	MOTA	3980	C	ARG	189	8.905	12.499	64.357	1.00 61.00	В
70	MOTA	3981	0	ARG	189	7.952	11.725	64.399	1.00 61.27	В
70	MOTA	3982	N	ASN	190	10.159	12.118	64.590	1.00 63.40	₿
	MOTA	3983	CA	ASN	190	10.516	10.735	64.914	1.00 65.21	В
	MOTA	3984	CB.	ASN	190	10.752	9.935	63.625	1.00 65.05	В
	ATOM	3985	CG	ASN	190	11.750	10.604	62.692	1.00 64.67	В
										-

		2006								_
	MOTA	3986		ASN	190	12.954	10.474	62.861	1.00 64.77	В
	ATOM ATOM	3987 3988		ASN	190 190	11.242	11.332 10.684	61.707	1.00 63.52	В
	ATOM	3989	C	ASN ASN	190	11.757 12.850	11.038	65.807 65.381	1.00 66.41 1.00 66.57	· B B
5	ATOM	3990	N	LYS	191	11.575	10.241	67.051	1.00 67.89	В
•	MOTA	3991	CA.	LYS	191	12.676	10.158	68.017	1.00 68.02	В
	ATOM	3992	CB	LYS	191	12.151	9.687	69.378	1.00 69.77	В
	ATOM	3993	CG	LYS	191	11.151	10.636	70.012	1.00 71.09	В
	ATOM	3994	CD	LYS	191	11.787		70.297	1.00 72.77	В
10	MOTA	3995	CE	LYS	191	10.771	12.963	70.860	1.00 74.00	В
	ATOM	3996	NZ	LYS	191	9.657	13.210	69.902	1.00 75.27	ъ в
	ATOM	3997	С	LYS	191	13.826	9.251	67.571	1.00 66.64	В
	MOTA	3998	0	LYS	191	14.852	9.149	68.253	1.00 66.18	В
15	MOTA	3999	·N	ARG	192	13.641	8.587	66.434	1.00 64.41	В
15	ATOM	4000	CA	ARG	192	14.668	7.720	65.878	1.00 62.32	В
	ATOM	4001	CB	ARG	192	14.101	6.946	64.685	1.00 64.84	. В
	ATOM	4002	CG	ARG	192	15.134	6.138	63.909	1.00 68.49	В
	MOTA MOTA	4003 4004	CD NE	ARG ARG	192 192	14.582 14.312	5.584 6.616	62.578 61.569	1.00 71.52 1.00 73.79	B B
20	ATOM	4005	CZ	ARG	192	13.207	7.359	61.506	1.00 74.82	В
	ATOM	4006		ARG	192	12.232	7.201	62.393	1.00 75.36	B
	ATOM	4007		ARG	192	13.079	8.275	60.555	1.00 75.53	В
	ATOM	4008	С	ARG	192	15.822	8.612	65.403	1.00 59.33	В
	ATOM	4009	ŏ	ARG	192	16.991	8.235	65.479	1.00 58.48	B
25	ATOM	4010	N	GLY	193	15.468	9.805	64.927	1.00 55.93	В
	MOTA	4011	CA	GLY	193	16.453	10.747	64.429	1.00 50.05	. В
	MOTA	4012	С	GLY	193	16.778	11.895	65.364	1.00 45.96	В
	ATOM	4013	0	GLY	193	16.345	11.933	66.518	1.00 44.90	В
30	MOTA	4014	N	VAL	194	17.547	12.842	64.839	1.00 42.75	В
30	ATOM	4015	CA	VAL	194	17.968	14.006	65.596	1.00 39.18	В
	ATOM ATOM	4016 4017	CB	VAL VAL	194 194	19.328 20.450	13.743 13.925	66.269 65.262	1.00 39.02 1.00 38.70	B B
	ATOM	4018		VAL	194	19.504	14.653	67.456	1.00 38.46	В
	ATOM	4019	c	VAL	194	18.096	15.209	64.666	1.00 37.27	В
35	MOTA	4020	Ō	VAL	194	18.181	15.057	63.456	1.00 36.48	В.
	MOTA	4021	N	ILE	195	18.108	16.400	65.254	1.00 35.15	В
	MOTA	4022	CA	ILĘ	195	18.230	17.645	64.501	1.00 33.17	В
	MOTA	4023	CB	ILE	195	17.002	18.543	64.702	1.00 34.99	В
40	MOTA	4024		ILE	195	17.185	19.842	63.916	1.00 36.47	В
40	MOTA	4025		ILE	195	15.731	17.803	64.280	1.00 36.88	В
	MOTA MOTA	4026 4027	CDI	ILE	195 195	15.658 19.452	17.513 18.465	62.784 64.917	1.00 38.32 1.00 30.37	B B
	MOTA	4028	õ	ILE	195	19.575	18.870	66.063	1.00 30.37	В
	ATOM	4029	N	ILE	196	20.353	18.711	63.975	1.00 28.58	В
45	ATOM	4030	CA	ILE	196	21.538	19.503	64.270	1.00 27.51	В
	ATOM	4031	CB	ILE	196	22.810	18.928	63.572	1.00 26.71	В
	ATOM	4032	CG2	ILE	196	24.024	19.795	63.884	1.00 25.48	В
	MOTA	4033	CG1	ILE	196	23.107	17.515	64.078	1.00 25.19	В
50	MOTA	4034	CD1	ILE	196	22.263	16.456	63.472	1.00 25.37	В
50	MOTA	4035	C	ILE	196	21.284	20.931	63.787	1.00 27.55	В
	MOTA	4036	0	ILE	196	21.307	21.212	62.601	1.00 27.49	В
	MOTA MOTA	4037 4038	N CA	LYS LYS	197 197	21.045 20.765	21.832 23.229	64.730	1.00 28.27	В
	ATOM	4039	CB	LYS	197	20.765	23.223	64.418 65.688	1.00 27.24	B B
55	MOTA	4040	CG	LYS	197	19.970	25.451	65.508	1.00 26.93	В
	ATOM	4041	CD	LYS	197	19.665	26.075	66.853	1.00 27.21	В
	ATOM	4042	CE	LYS	197	19.417	27.563	66.750	1.00 26.28	В
	ATOM	4043	NZ	LYS	197	19.153	28.144	68.104	1.00 26.63	В
60	MOTA	4044	С	LYS	197	21.961	23.947	63.821	1.00 26.61	В
60	ATOM	4045	0	LYS	197	23.039	23.974	64.406	1.00 27.65	В
	MOTA	4046	N	GLY	198	21.762	24.513	62.637	1.00 26.31	В
	ATOM	4047	CA	GLY	198	22.826	25.266	61.998	1.00 25.56	В
	MOTA MOTA	4048 4049	0	GLY GLY	198 198	23.747 24.518	24.536 25.162	61.044. 60.335	1.00 24.60	В
65	ATOM	4050	N	LEU	199	23.680	23.162	61.029	1.00 24.69 1.00 25.09	B B
	ATOM	4051	CA	LEU	199	24.523	22.433	60.130	1.00 25.50	В
	ATOM	4052	CB	LEU	199	24.357	20.927	60.411	1.00 24.64	В
	MOTA	4053	CG	LEU	199	25.219	19.950	59.597	1.00 24.37	В
7 0	MOTA	4054		LEU	199	26.699	20.274	59.742	1.00 22.90	В
70	MOTA	4055		LEU	199	24.942	18.535	60.068	1.00 23.77	В
	MOTA	4056	C	LEU	199	24.235	22.767	58.648	1.00 25.50	В
	MOTA	4057	0	LEU	199	23.160	22.510	58.114	1.00 24.77	В
	MOTA	4058	N	GLU	200	25.225	23.350	57.991	1.00 26.00	В

	MOTA	4059	CA	GLU	200 200	25.087 26.274	23.722 24.568	56.598 56.143	1.00 26.47	В
	ATOM ATOM	4060 4061	CB	GLU GLU	200	26.274	25.971	56.724	1.00 27.75 1.00 32.47	B B
	ATOM	4062	CD	GLU	200	25.112	26.821	56.339	1.00 35.25	В
5	ATOM	4063		GLU	200	24.061	26.700	57.004	1.00 38.07	В
	ATOM	4064		GLU	200	25.196	27.600	55.363	1.00 35.41	В
	ATOM		C	GLU	200	25.029	22.508	55.686	1.00 27.12	В
	MOTA	4066	0	GLU	200	25.586	21.457	55.972	1.00 26.69	В
10	ATOM	4067	N	GLU	201	24.327	22.678	54.579	1.00 27.51	В
10	ATOM	4068	CA	GLU	201	24.218	21.646	53.574	1.00 26.72	В
	MOTA	4069	CB	GLU	201	22.790	21.135	53.468	1.00 27.33	В
	ATOM ATOM	4070 4071	CD	GLU	201 201	22.239 · 20.954	20.532 19.773	54.722 54.457	1.00 30.03	B
•	ATOM	4072		GLU	201	20.075	19.784	55.345	1.00 34.01	В
15	MOTA	4073		GLU	201	20.817	19.167	53.367	1.00 33.38	В
	MOTA	4074	С	GLU	201	24.581	22.363	52.278	1.00 26.18	В
	MOTA	4075	0	GLU	201	23.866	23.259	51.853	1.00 25.94	В
	MOTA	4076	N	ILE	202	25.707	21.996	51.674	1.00 25.78	В
20	MOTA	4077	CA	ILE	202	26.116	22.631	50.433	1.00 25.80	В
20	MOTA MOTA	4078 4079	CB	ILE	202 202	27.636 28.022	22.813 23.102	50.360 48.914	1.00 25.61 1.00 25.19	. В В
	ATOM	4080	CG1	ILE	202	28.089	23.969	51.258	1.00 26.32	В
	ATOM	4081	CD1	ILE	202	27.704	23.871		1.00 25.98	В.
	MOTA	4082	С	ILE	202	25.655	21.820	49.231	1.00 26.76	·B
25	MOTA	4083	0	ILE	202	25.798	20.597	49.195	1.00 26.87	В
	MOTA	4084	N	THR	203	25.089	22.508	48.248	1.00 26.89	В
	ATOM	4085	ÇA	THR	203	24.610	21.817	47.070	1.00 28.63	В
	MOTA MOTA	4086 4087	CB OG1	THR THR	203 203	23.463	22.606 22.683	46.329 47.167	1.00 28.93 1.00 28.96	B
30	ATOM	4088	CG2	THR	203	23.103	21.922	44.987	1.00 25.61	В
-	ATOM	4089	c	THR	203	25.774	21.634	46.120	1.00 29.69	В
	ATOM	4090	ō	THR	203	26.546	22.547	45.906	1.00 31.36	В
·	MOTA	4091	N	VAL	204	25.919	20.428	45.589	1.00 30.40	В
25.	ATOM	4092	CA	VAL	204	26.967	20.168	44.620	1.00 30.44	В
35 ⁻	ATOM ·	.4093	CB	VAL	204	27.656	18.798	44.876	1.00 29.19	В
•	ATOM ATOM	4094 4095		VAL VAL	204	28.839 28.142	18.609 18.733	43.930 46.292	1.00 28.81	В
	ATOM	4096	C	VAL	204 204	26.142	20.159	43.277	1.00 29.07	B B
	MOTA	4097	Ö	VAL	204	25.536	19.180	42.956	1.00 31.70	В
40	ATOM	4098	N	HIS	205	26.354	21.255	42.521	1.00 31.11	В
	ATOM	4099	CA	HIS	205	25.709	21.420	41.214	1.00 30.37	В
	MOTA	4100	CB	HIS	205	25.803	22.869	40.792	1.00 29.29	В
	ATOM	4101	CG	HIS	205	25.131	23.788	41.747	1.00 29.35	В
45	ATOM ATOM	4102 4103		HIS HIS	205 205	25.631 23.760	24.594 23.890	42.712 41.831	1.00 29.07 1.00 29.17	B B
45	MOTA	4104		HIS	205	23.444	24.721	42.806	1.00 29.17	В
	ATOM	4105		HIS	205	24.561	25.161	43.357	1.00 29.64	В
	ATOM	4106	С	HIS	205	26.252	20.533	40.100	1.00 30.88	В
50	MOTA	4107	Ο.	HIS	205	25.508	20.130	39.216	1.00 31.82	В
50	MOTA	4108	N	ASN	206	27.544	20.238	40.138	1.00 29.74	В
	MOTA	4109 4110	CA CB	ASN ASN	206 206	28.127 28.377	19.370 20.158	39.141 37.852	1.00 29.11 1.00 28.48	В
	MOTA MOTA	4111	CG	ASN	206	29.156	21.438	38.091	1.00 28.48	. В В
	MOTA	4112		ASN	206	30.252	21.412	38.645	1.00 28.71	В
55	MOTA	4113		ASN	206	28.594	22.562	37.673	1.00 28.54	В
	MOTA	4114	С	ASN	206	29.387	18.760	39.729	1.00 28.47	В
	MOTA	4115	0	ASN	206	29.740	19.032	40.852	1.00 27.98	В
	ATOM	4116	N	LYS	207	30.063	17.924	38.957	1.00 29.11	В.
60	MOTA	4117	CA	LYS	207	31.274	17.291	39.445	1.00 30.00	В
ŲŪ	ATOM ATOM	4118 4119	CB	LYS LYS	207 207	31.662 32.257	16.107 16.495	38.553 37.222	1.00 30.11 1.00 32.75	B B
	MOTA	4120	CD	LYS	207	32.719	15.270	36.441	1.00 32.75	В
	ATOM	4121	CE	LYS	207	33.466	15.669	35.164	1.00 34.56	B
	MOTA	4122	NZ	LYS	207	34.775	16.370	35.404	1.00 33.30	В
65	MOTA	4123	C	LYS	207	32.425	18.293	39.488	1.00 30.73	В
	MOTA	4124	0	LYS	207	33.458	18.026	40.089	1.00 32.12	В
	MOTA	4125	N	ASP	208	32.241	19.451	38.863	1.00 29.02	В
	ATOM	4126 4127	CA	ASP	208 208	33.301 33.234	20.453	38.850	1.00 28.26	В
70	MOTA MOTA	4127	CB	ASP ASP	208	33.234	21.261 20.463	37.556 36.354	1.00 31.08 1.00 32.65	B B
	ATOM	4129		ASP	208	33.702	20.729	35.233	1.00 32.03	В
	ATOM	4130		ASP	208	34.567	19.570	36.523	1.00 33.75	В
	ATOM	4131	С	ASP	208	33.277	21.374	40.065	1.00 26.42	В

	MOTA	4132	0	ASP	208	33.989	22.372	40.117	1.00 24.98	В
	MOTA	4133	N	GLU	209	32.462	21.032	41.052	1.00 25.24	В
	MOTA	4134	CA	GLU	209	32.388	21.831	42.272	1.00 25.22	. В
5	MOTA	4135	CB	GLU	209	30.958	22.278	42.595	1.00 27.01	В
J	ATOM	4136	CG	GLU	209	30.306	23.237	41.602	1.00 30.48	В
	ATOM	4137	CD	GLU	209	29.069	23.926	42.167	1.00 32.55	В
	ATOM	4138	OE1		209	28.371	24.610	41.385	1.00 34.80	В
	ATOM	4139	OE2		209	28.804	23.793	43.382	1.00 33.17	В
10	ATOM	4140	C	GLU	209	32.832		43.490	1.00 24.23	В
10	ATOM	4141	0	GLU	209	33.194	21.596	44.513	1.00 25.15	В
	MOTA	4142	N	VAL	210	32.835	19.708	43.373	1.00 21.99	• В
	MOTA	4143	CA	VAL	210	33.205	18.882	44.514	1.00 18.98	В
	MOTA	4144	CB	VAL VAL	210	32.987 32.238	17.360 17.180	42.928	1.00 17.62	В
15	MOTA MOTA	4145 4146		VAL	210 210	34.290	16.638	44.159	1.00 17.92 1.00 17.49	B B
13	ATOM	4147	C	VAL	210	34.609	19.093	45.082	1.00 17.49	В
	MOTA	4148		VAL	210	34.775	19.138	46.289	1.00 19.29	. В
	ATOM	4149	N	TYR	211	35.620	19.238	44.232	1.00 17.72	В
	ATOM	4150	CA	TYR	211	36.968	19.401	44.770	1.00 15.84	В
20	ATOM	4151	СВ	TYR	211	38.030	19.361	43.656	1.00 14.23	В
	ATOM	4152	CG	TYR	211	39.441	19.224	44.196	1.00 13.57	B
	ATOM	4153		TYR	211	39.807	18.110	44.937	1.00 12.81	В
	ATOM	4154		TYR	211	41.062	18.018	45.528	1.00 12.54	В
	MOTA	4155	CD2	TYR	211	40.379	20.246	44.048	1.00 14.65	В
25	ATOM	4156		TYR	211	41.651	20.166	44.642	1.00 13.74	·B
	ATOM	4157	CZ	TYR	211	41.987	19.048	45.386	1.00 14.45	. В
	ATOM	4158	ОН	TYR	211	43.235	18.972	45.997	1.00 10.15	В
	ATOM	4159	C	TYR	211	37.083	20.665	45.608	1.00 15.70	В
	MOTA	4160	ō	TYR	211	37.626	20.620	46.696	1.00 14.92	В
30	ATOM	4161	N	GLN	212	36.557	21.781	45.101	1.00 17.75	В
	ATOM	4162	CA	GLN	212	36.582	23.064	45.819	1.00 18.64	В
		4163	СВ	GLN	212	35.897	24.154	44.983	1.00 19.40	В
	ATOM	4164	CG	GLN	212	35.962	25.543	45.607	1.00 24.51	В
	ATOM	4165	CD	GLN	212	35.764	26.672	44.587	1.00 26.82	В
35	MOTA	4166	OE1	GLN	212	35.046	26.508	43.594	1.00 25.33	В
	MOTA	4167	NE2	GLN	212	36.391	27.832	44.844	1.00 26.86	В
	MOTA	4168	C	GLN	212	35.909	22.923	47.192	1.00 18.53	В
	MOTA	4169	0	GLN	212	36.420	23.374	48.193	1.00 19.69	В
40	ATOM	4170	N	ILE	213	34.759	22.265	47.230	1.00 19.83	В
40	ATOM	4171	CA	ILE	213	34.031	22.048	48.485	1.00 19.97	В
	ATOM	4172	CB	ILE	213	32.664	21.350	48.237	1.00 20.59	В
	MOTA	4173		ILE	213	32.022	20.933	49.579	1.00 19.77	В
	MOTA	4174		ILE	213	31.758	22.285	47:441	1.00 20.66	В
45	MOTA	4175		ILE	213	30.505	21.626	46.928	1.00 22.87	В
45	MOTA	4176	С	ILE	213	34.831	21.189	49.461	1.00 20.10	В
	MOTA	4177	0	ILE	213	34.822	21.446	50.672	1.00 20.46	В
	MOTA	4178	N	LEU	214	35.489	20.156	48.937	1.00 19.00	В
	MOTA	4179	CA	LEU	214	36.310	19.282	49.759	1.00 18.96	В
50	ATOM	4180	CB	LEU	214	36.829	18.100	48.950	1.00 18.27	В
50	MOTA	4181	CG	LEU	214	36.013	16.826	49.015	1.00 18.28	В
	MOTA	4182		LEU	214	34.547	17.179	48.926	1.00 22.38	В
	MOTA	4183		LEU	214	36.443	15.908	47.895	1.00 17.95	В
	ATOM	4184	C	LEU	214	37.507	20.048	50.316	1.00 19.17	В
55	ATOM	4185	0	LEU	214	37.920	19.821	51.443	1.00 20.21	В
55	ATOM	4186	N	GLU	215	38.055	20.967	49.523	1.00 19.88	В
	MOTA	4187 4188	CA	GLU	215	39.208	21.768	49.953	1.00 19.18	В
	ATOM	4189	CB	GLU	215	39.748	22.628	48.797	1.00 19.26	В
	MOTA		CG	GLU	215	40.496	21.863	47.699	1.00 20.08	В
60	ATOM	4190	CD	GLU	215	41.103	22.786	46.630	1.00 20.78	' В
00	MOTA MOTA	4191 4192	OE2	GLU	215 215	42.352 40.337	22.898 23.399	46.580 45.842	1.00 16.87 1.00 19.38	В
	ATOM	4193	C	GLU	215	38.855	22.700	51.110	1.00 19.38	В
	ATOM	4194	ò	GLU	215	39.592	22.798	52.092	1.00 17.36	В
	MOTA	4195	N	LYS	216	37.732	23.397	50.988	1.00 17.38	B
65	ATOM	4196	CA	LYS	216	37.732	24.300	52.042	1.00 19.53	B B
55	ATOM	4197	CB	LYS	216	35.993	24.300	51.620	1.00 20.63	B
	ATOM	4198	CG	LYS	216	36.240	26.094	50.602	1.00 22.77	В
	ATOM	4199	CD	LYS	216	34.962	26.743	50.069	1.00 23.39	В
	ATOM	4200	CE	LYS	216	35.281	27.963	49.187	1.00 35.20	В
70	ATOM	4201	NZ	LYS	216	36.198	27.671	48.028	1.00 37.67	В
, -	ATOM	4202	C	LYS	216	37.144	23.547	53.361	1.00 20.03	. B
	ATOM	4203	õ	LYS	216	37.501	24.057	54.416	1.00 20.03	. В
	ATOM	4204	N	GLY	217	36.628	22.329	53.309	1.00 18.86	В
										_

•	MOTA	4205	CA	GLY	217	36.492	21.587	54.543	1.00 18.29	В
	MOTA	4206	С	GLY	217	37.869	21.334	55.128	1.00 18.39	В
	MOTA	4207	ō	GLY	217	38.103	21.531	56.307	1.00 18.74	В
_	MOTA	4208	N	ALA	218	38.792	20.895	54.282	1.00 19.27	В
5	MOTA	4209	CA	ALA	218	40.148	20.607	54.737	1.00 19.03	В
	MOTA	4210	CB	ALA	218	40.996	20.061	53.580	1.00 18.52	В
	ATOM	4211	c	ALA	218	40.827	21.818	55.363	1.00 18.17	B
•	MOTA	4212	0	ALA	218	41.470	21.706	56.403	1.00 19.12	В
	MOTA	4213	N	ALA	219	40.691	22.980	54.735	1.00 17.99	В
10	ATOM	4214	CA	ALA	219	41.315	24.203	55.266	1.00 16.17	В
	MOTA	4215	·CB	ALA	219	41.044	25.404	54.323	1.00 14.07	В
	MOTA	4216	С	ALA	219	40.792	24.505	56.671	1.00 14.78	В
	MOTA	4217	0	ALA	219	41.552	24.760	57.599	1.00 15.56	В
	ATOM	4218	N	LYS	220	39.479	24.450	56.823	1.00 14.00	В
15	ATOM	4219			220			58.110	1.00 13.80	
IJ			CA	LYS		38.859	24.729			В
	MOTA	4220	CB	LYS	220	37.338	24.667	57.978	1.00 11.84	В
	MOTA	4221	CG	LYS	220	36.603	25.222	59.177	1.00 12.63	В
	MOTA	4222	CD	LYS	220	35.130	25.462	58.884	1.00 11.67	В
	MOTA	4223	CE	LYS	220	34.464	26.087	60.092	1.00 13.88	В
20										
20	MOTA	4224	NZ	LYS	220	32.993	26.287	59.939	1.00 12.51	. В
	MOTA	4225	C .	LYS	220	39.303	23.734	59.173	1.00 14.26	В
	ATOM	4226	0	LYS	220	39.442	24.067	60.350	1.00 15.25	В
	MOTA	4227	N	ARG	221	39.513	22.498	58.748	1.00 14.19	B
25	MOTA	4228	CA	ARG	221	39.936	21.438	59.647	1.00 11.64	В
25	MOTA	4229	CB	ARG	221	39.878	20.111	58.889	1.00 13.12	В
	MOTA	4230	CG	ARG	221	40.038	18.857	59.751	1.00 13.06	В
	ATOM	4231	CD	ARG	221	39.999	17.586	58.902	1.00 11.48	В
	MOTA	4232	NE	ARG	221	38.638	17.093	58.691		В
20	MOTA	4233	CZ	ARG	221	38.317	16.184	57.774	1.00 8.38	В
30	MOTA	4234	NH1	ARG	221	39.255	15.687	56.976	1.00 5.16	В
	ATOM	4235	NH2	ARG	221	37.074	15.732	57.687	1.00 8.15	B
	MOTA	4236	c	ARG	221	41.345	21.737	60.174	1.00 10.67	B
	MOTA	4237	0	ARG	221	41.686	21.394	61.314	1.00 10.15	В
~ =	MOTA	4238	N	THR	222	42.167	22.372	59.342	1.00 10.52	В
35	MOTA	. 4239	CA	THR	222	43.515	22.747	59.752	1.00 7.37	В
	ATOM	4240	CB	THR	222	44.277	23.438	58.634	1.00 6.75	В
	MOTA	4241	OG1		222	44.586	22.466	57.637	1.00 9.09	В
	MOTA	4242	CG2	THR	222	45.573 .	24.026	59.136	1.00 5.92	В
	MOTA	4243	С	THR	222	43.475	23.692	60.916	1.00 5.52	В
40	ATOM	4244	0	THR	222	44.265	23.598	61.797	1.00 6.41	В
	MOTA	4245	N		223					
				THR		42.527	24.607	60.906	1.00 5.73	В
	ATOM	4246	CA	THR	223	42.443	25.550	61.990	1.00 7.41	В
	MOTA	4247	CB	THR	223	41.481	26.706	61.654	1.00 9.80	В
	ATOM	4248	OG1	THR	223	40.126	26.260	61.807	1.00 13.96	В
45	ATOM	4249		THR	223	41.716	27.205	60.212	1.00 11.03	В
73										
	MOTA	4250	С	THR	223	41.941	24.801	63.206	1.00 8.79	В
	MOTA	4251	0	THR	223	42.353	25.101	64.337	1.00 11.00	В
	ATOM	4252	N	ALA	224	41.093	23.796	62.970	1.00 9.46	В
	ATOM	4253	CA:	ALA	224	40.537	23.001	64.069	1.00 9.41	В
50	ATOM	4254	CB	ALA		39.514				
50					224		21.966	63.570	1.00 8.72	В
	MOTA	4255	С	ALA	224	41.645	22.288	64.798	1.00 10.87	В
	MOTA	4256	0	ALA	224	41.693	22.258	66.041	1.00 10.92	В
	ATOM	4257	N	ALA	225	42.526	21.678	64.020	1.00 11.03	В
	MOTA	425B	CA	ALA	225	43.647	20.977	64.608	1.00 10.24	В
55										
JJ	MOTA	4259	CB	ALA	225	44.484	20.347	63.517	1.00 9.24	В
	MOTA	4260	С	ALA	225	44.502	21.942	65.446	1.00 11.63	В
	MOTA	4261	0	ALA	225	44.983	21.592	66.516	1.00 12.58	В
	MOTA	4262	N	THR	226	44.676	23.164	64.957	1.00 13.45	В.
	ATOM	4263	CA	THR	226	45.490	24.156	65.650	1.00 15.18	
60 ·										В
OO .	MOTA	4264	CB	THR	226	45.557	25.470	64.868	1.00 14.69	В
	ATOM	4265	OG1	THR	226	46.323	25.286	63.670	1.00 16.29	В
	MOTA	4266		THR	226	46.186	26.534	65.716	1.00 15.17	В
	MOTA	4267	C	THR	226	44.901	24.452	67.007	1.00 16.64	B
65	MOTA	4268	0	THR	226	45.617	24.553	67.998	1.00 16.41	В
65	MOTA	4269	N	LEU	227	43.575	24.575	67.025	1.00 18.18	В
	MOTA	4270	CA	LEU	227	42.805	24.875	68.238	1.00 18.74	В
	MOTA	4271	СВ	LEU	227	41.367	25.310	67.899	1.00 19.87	В
	MOTA	4272	CG		227			68.051		
				LEU		40.955	26.772		1.00 21.86	В
70	MOTA	4273		LEU	227	41.103	27.134	69.518	1.00 21.93	В
70	MOTA	4274	CD2	LEU	227	41.786	27.693	67.155	1.00 21.51	В
	ATOM	4275	С	LEU	227	42.651	23.733	69.239	1.00 18.17	В
	MOTA	4276	õ	LEU	227	42.783	23.928	70.435	1.00 18.61	
										В
	MOTA	4277	N	MET	228	42.380	22.536	68.742	1.00 18.27	В

•	ATOM	4278	CA	MET	228	42.160	21.404	69.634	1.00 17.51	В
	ATOM	4279	CB	MET	228	40.800	20.772	69.302	1.00 16.30	В
	ATOM	4280	CG	MET	228	39.649	21.745	69.495	1.00 16.20	В
	MOTA	4281	SD	MET	228	38.056	21.201	68.874	1.00 19.18	В
5	ATOM	4282	CE	MET	228					
,						38.092	22.153	67.250	1.00 17.21	В
	ATOM	4283	C	MET	228	43.250	20.342	69.614	1.00 18.14	В
	ATOM	4284	0	MET	228	43.769	19.990	68.549	1.00 20.11	• В
	MOTA	4285	N	ASN	229	43.571	19.834	70.807	1.00 16.66	В
	MOTA	4286	CA	ASN	229	44.589	18.799	70.992	1.00 16.35	В
10	MOTA	4287	CB	ASN	229	44.824	18.543	72.485	1.00 15.94	В
	ATOM	4288	CG	ASN	229	45.350	19.764	73.209	1.00 16.33	В
	ATOM	4289		ASN	229	45.764	20.739	72.588	1.00 17.78	В
	MOTA	4290		ASN	229	45.340	19.711	74.534	1.00 14.68	В
	MOTA	4291	С	ASN	229	44.311	17,448	70.313	1.00 15.68	В
15	MOTA	4292	0	ASN	229	43.228	16.873	70.460	1.00 15.38	В
	MOTA	4293	N	ALA	230	45.300	16.950	69.569	1.00 14.15	В
	ATOM	4294	CA	ALA	230	45.171	15.679	68.863	1.00 12.00	В
	MOTA	4295	СВ	ALA	230	45.241	14.546	69.847	1.00 11.64	В
20	MOTA	4296	C	ALA	230	43.869	15.595	68.079	1.00 11.58	В
20	ATOM	4297	0	ALA	230	43.269	14.519	67.977	1.00 10.16	В
	MOTA	4298	N	TYR	231	43.443	16.725	67.519	1.00 11.27	В
	MOTA	4299	CA	TYR	231	42.200	16.775	66.761	1.00 12.69	В.
	ATOM	4300	CB	TYR	231	42.047	18.119	66.029	1.00 11.10	В
	MOTA	4301	CG	TYR	231	40.667	18.312	65.435	1.00 10.24	·B
25	ATOM	4302	CD1		231	40.404	17.998	64.112	1.00 9.88	В
	ATOM	4303	CE1		231	39.121	18.122	63.598	1.00 10.11	
										В
	MOTA	4304	CD2	TYR	231	39.606	18.760	66.229	1.00 11.37	В
	MOTA	4305	CEZ	TYR	231	38.316	18.886	65.716	1.00 10.13	В
20	MOTA	4306	CZ	TYR	231	38.079	18.559	64.402	1.00 9.90	· В
30	ATOM	4307	он	TYR	231	36.780	18.623	63.936	1.00 7.41	В
	ATOM	4308	С	TYR	231	41.988	15.645	65.748	1.00 13.47	В
	MOTA	4309	0	TYR	231	41.016	14.916	65.837	1.00 14.47	В
	ATOM	4310	N	SER	232	42.904	15.481	64.800	1.00 15.55	В
	ATOM	4311	CA	SER	232	42.744	14:446	63.777	1.00 15.70	
35 ·										В
55	ATOM	4312	CB	SER	232	43.907	14.490	62.779	1.00 17.08	В
	MOTA	4313	OG	SER	232	45.145	14.290	63.419	1.00 20.92	В
	MOTA	4314	С	SER	232	42.60B	13.020	64.308	1.00 15.28	В
	ATOM	4315	0	SER	232	41.898	12.203	63.726	1.00 16.22	В
	ATOM	4316	N	SER	233	43.260	12.711	65.417	1.00 12.45	В
40	MOTA	4317	CA	SER	233	43.173	11.352	65.919	1.00 12.60	В
. •	MOTA	4318	CB	SER	233	44.477	10.942	66.596	1.00 13.54	В
	ATOM	4319	OG		233					
				SER		44.662	11.602	67.838	1.00 15.82	В
	MOTA	4320	Ç	SER	233	42.057	11.167	66.921	1.00 12.47	В
45	MOTA	4321	0	SER	233	41.604	10.047	67.155	1.00 12.18	В
45	MOTA	4322	N	ARG	.234	41.612	12.265	67.523	1.00 11.28	В
	MOTA	4323	CA	ARG	234	40.558	12.168	68.532	1.00 9.69	В
	MOTA	4324	CB	ARG	234	40.919	12.961	69.784	1.00 10.96	В
	MOTA	4325	CG	ARG	234	41.315	12.112	70.975	1.00 13.22	В
	ATOM	4326	CD	ARG	234	42.707	12.435	71.494	1.00 16.77	B
50	ATOM	4327	NE	ARG	234	42.755	13.676	72.263		
50		4328	CZ						1.00 20.42	В
	MOTA			ARG	234	43.751	14.005	73.083	1.00 22.86	₿
	MOTA	4329	NH1	ARG	234 .	44.791	13.186	73.242	1.00 22.37	В
	MOTA	4330	NH2	ARG	234	43.690	15.140	73.767	1.00 25.64	В
	MOTA	4331	C	ARG	234	39.168	12.617	68.118	1.00 7.73	В
55	ATOM	4332	0	ARG	234	38.258	12.599	68.924	1.00 8.22	В
	ATOM	4333	N	SER	235	39.006	13.014	66.862	1.00 6.52	В
	MOTA	4334	CA	SER	235	37.697	13.455	66.394	1.00 4.31	В
		4335				37.785	14.801	65.647		
	ATOM		CB	SER	235				1.00 2.24	₿.
ζΛ .	MOTA	4336	OG	SER	235	38.745	14.780	64.602	1.00 1.00	В
60 ·	MOTA	4337	C	SER	235	37:048	12.437	65.488	1.00 2.58	В
	MOTA	4338	0	SER	235	37.704	11.648	64.854	1.00 3.58	B
	MOTA	4339	N	HIS	236	35.725	12.465	65.472	1.00 4.87	В
	ATOM	4340	CA	HIS	236	34.911	11.587	64.631	1.00 5.05	B
	MOTA	4341	СВ	HIS	236	33.691	11.087	65.386	1.00 4.65	В
65	ATOM	4342	CG	HIS	236					
5 5						34.032	10.280	66.586	1.00 4.01	В
	MOTA	4343	CD2		236	34.066	10.607	67.899	1.00 3.63	В
	MOTA	4344		HIS	236	34.437	8.965	66.504	1.00 3.84	В
	ATOM	4345		HIS	236	34.704	8.517	67.717	1.00 4.48	В
	MOTA	4346	NE2	HIS	236	34.487	9.494	68.582	1.00 4.72	В
70	MOTA	4347	С	HIS	236	34.347	12.498	63.556	1.00 6.99	В
-	ATOM	4348	ō	HIS	236	33.810	13.556	63.878	1.00 9.70	В
	ATOM	4349	Ñ.	SER	237	34.475	12.108	62.291		
									1.00 7.23	В
	MOTA	4350	CA	SER	237	33.951	12.933	61.208	1.00 6.69	В

	ATOM	4351	СВ	SER	237	35.058	13.406	60.253	1.00 5.37	В
	ATOM	4352	ŌĞ	SER	237	35.464	12.358	59.380	1.00 3.60	В
	ATOM	4353	C	SER	237	32.946	12.157	60.393	1.00 7.89	В
_	MOTA	4354	0	SER	237	33.196	11.040	59.976	1.00 9.95	В
5	MOTA	4355	N	VAL	238	31.787	12.753	60.180	1.00 7.91	B
	MOTA	4356	CA	VAL	238	30.787	12.078	59.392	1.00 7.74	В
	MOTA	4357	CB	VAL	238	29.560	11.740	60.282	1.00 8.04	В
	ATOM	4358		VAL	238	29.413	12.787	61.328	1.00 7.80	В
10	MOTA	4359		VAL	238	28.307		59.460	1.00 8.71	В
10	MOTA MOTA	4360 4361	C	VAL VAL	238 238	30.421	12.935	58.182	1.00 8.25	В
	ATOM	4362	N	PHE	239	29.776 30.883	13.952 12.511	58.323 57.002	1.00 9.09 1.00 8.31	· В
	ATOM	4363	CA	PHE	239	30.609	13.198	55.732	1.00 8.81	B B
	ATOM	4364	CB	PHE	239	31.793	13.036	54.759	1.00 6.73	B
15	MOTA	4365	CG	PHE	239	31.693	13.893	53.525	1.00 6.12	В
	MOTA	4366	CD1	PHE	239	30.815	13.557	52.500	1.00 5.69	В
	MOTA	4367	CD2	PHE	239	32.462	15.046	53.394	1.00 5.95	· B
	ATOM	4368		PHE	239	30.705	14.364	51.348	1.00 5.30	В
20	ATOM	4369		PHE	239	32.354	15.854	52.247	1.00 5.11	В
20	MOTA	4370	cz	PHE	239	31.475	15.511	51.224	1.00 3.58	В
	MOTA	4371	C	PHE	239	29.350	12.553	55.148	1.00 9.90	В
	MOTA MOTA	4372 4373	O N	PHE	239 240	29.327	11.356	54.859	1.00 9.81	В
	MOTA	4374	CA	SER	240	28.305 27.039	13.359 12.871	54.982 54.466	1.00 10.63	В
25	ATOM	4375	CB	SER	240	25.926	13.194	55.467	1.00 9.05 1.00 9.24	B B
	ATOM	4376	OG	SER	240	26.182	12.631	56.742	1.00 8.98	В
	MOTA	4377	C	SER	240	26.678	13.462	53.105	1.00 10.23	В
	MOTA	4378	0	SER	240	26.809	14.668	52.877	1.00 10.82	В
20	MOTA	4379	N	VAL	241	26.230	12.601	52.198	1.00 10.77	В
30	MOTA	4380	CA	VAL	241	25.813	13.044	50.874	1.00 12.14	В
	ATOM	4381	CB	VAL	241	26.748	12.492	49.775	1.00 12.12	В
	MOTA	4382		VAL	241	26.981	11.008	50.002	1.00 13.27	В
	MOTA MOTA	4383 4384	CG2	VAL VAL	241 .	26.143	12.736	48.394	1.00 11.17	В
35	ATOM	4385	Ö	VAL	241 241	24.379 24.092	12.565 11.365	50.649 50.700	1.00 13.61	В
	ATOM	4386	Ŋ	THR	242	23.478	13.513	50.422	1.00 13.01	B B
	MOTA	4387	CA	THR	242	22.078	13.203	50.217	1.00 16.18	В
	MOTA	4388	CB	THR	242	21.198	14.104	51.118	1.00 17.52	В
40	MOTA	4389	OG1	THR	242	21.546	13.897	52.496	1.00 19.73	В
40	MOTA	4390	CG2	THR	242	19.738	13.766	50.954	1.00 20.46	В
	MOTA	4391	С	THR	242	21.746	13.418	48.741	1.00 18.15	В
	MOTA	4392	0	THR	242	22.212	14.357	48.128	1.00 19.20	В
	MOTA	4393	N	ILE	243	20.945	12.521	48.180	1.00 20.44	В
45	MOTA	4394	CA	ILE	243	20.560	12.619	46.785	1.00 23.13	В
73	MOTA MOTA	4395 4396	CB	ILE	243	21.178	11.477	45.941	1.00 22.27	В
	MOTA	4397		ILE	243 243	20.962 22.663	11.770	44.475	1.00 18.06	В
	ATOM	4398		ILE	243	23.247	11.310 10.072	46.270 45.722	1.00 21.29	B
	ATOM	4399	c	ILE	243	19.043	12.555	46.628	1.00 26.42	В
50	MOTA	4400	ō	ILE	243	18.442	11.488	46.790	1.00 27.92	В
	MOTA	4401	N	HIS	244	18.437	13.707	46.340	1.00 29.29	В
	MOTA	4402	CA	HIS	244	17.001	13.808	46.117	1.00 30.50	В
	MOTA	4403	CB	HIS	244	16.486	15.226	46.393	1.00 31.87	В
55	MOTA	4404	CG	HIS	244	16.375	15.565	47.845	1.00 34.67	В
JJ	MOTA MOTA	4405 4406	CD2		244	15.341	15.441	48.712	1.00 35.28	В
	MOTA	4407	ND1	HIS	244 244	17.424 17.040	16.087 16.267	48.577	1.00 36.67	В
	ATOM	4408	NE2		244	15.778	15.881	49.828 49.936	1.00 35.69 1.00 35.59	В
	ATOM	4409	C	HIS	244	16.803	13.494	44.637	1.00 33.39	B B
60	MOTA	4410	ŏ	HIS	244	17.277	14.228	43.755	1.00 32.44	В
	MOTA	4411	N	MET	245	16.122	12.388	44.368	1.00 32.37	В
	MOTA	4412	CA	MET	245	15.877	11.968	42.998	1.00 32.37	В
	MOTA	4413	CB	MET	245	16.475	10.578	42.791	1.00 31.86	В
65	MOTA	4414	CG	MET	245	17.968	10.548	43.055	1.00 31.73	В
UJ	ATOM	4415	SD	MET	245	18.589	8.875	43.225	1.00 33.02	В
	MOTA	4416	CE	MET .	245	18.034	8.477	44.892	1.00 31.10	В
	ATOM	4417	C	MET	245	14.401	12.002	42.601	1.00 31.83	В
	MOTA MOTA	4418 4419	о О	MET LYS	245 246	13.509	11.738	43.415	1.00 31.92	В
70	MOTA	4420	CA	LYS	246	14.159 12.811	12.334 12.428	41.337 40.804	1.00 31.84 1.00 31.99	B
-	MOTA	4421	СВ	LYS	246	12.350	13.895	40.781	1.00 31.99	B
	MOTA	4422	CG	LYS	246	10.922	14.087	40.292	1.00 34.26	В
	MOTA	4423	CD	LYS	246	10.606	15.539	39.946	1.00 34.52	В

	•									
•	ATOM	4424	CE	LYS	246	10.646	16.433	41.173	1.00 36.15	В
	MOTA	4425	NZ	LYS	246	10.457	17.872	40.836	1.00 35.42	В
	MOTA	4426	С	LYS	246	12.761	11.870	39.382	1.00 31.58	В
5	ATOM	4427	0	LYS	246	13.439	12.358	38.480	1.00 30.24	В
J	ATOM	4428	N	GLU	247	11.967	10.824	39.196	1.00 31.71	В
	MOTA	4429	CA	GLU	247	11.808	10.238	37.874	1.00 30.99	В
	MOTA	4430	CB	GLU	247	12.337	8.801	37.855	1.00 32.21	В
	MOTA	4431	CG	GLU	247	11.815	7.897	38.961	1.00 33.61	В
10	MOTA MOTA	4432 4433	CD	GLU	247 247	12.672 12.420	6.647 5.841	39.115 40.037	1.00 35.27	В
10	ATOM	4434		GLU	247	13.609	6.469	38.307	1.00 35.63 1.00 35.39	8
	MOTA	4435	C	GLU	247	10.338	10.298	37.479	1.00 30.04	B B
	MOTA	4436	ŏ	GLU	247	9.448	10.169	38.317	1.00 29.68	В
	ATOM	4437	Ň	THR	248	10.083	10.513	36.197	1.00 28.13	В
15	ATOM	4438	CA	THR	248	8.716	10.591	35.720	1.00 26.83	В
	MOTA	4439	CB	THR	248	8.506	11.895	34.942	1.00 25.80	В
•	MOTA	4440	0G1	THR	248	8.937	12.995	35.750	1.00 24.67	В
	MOTA	4441	CG2	THR	248	7.046	12.096	34.617	1.00 25.62	В
20.	MOTA	4442	C	THR	248	8.406	9.395	34.822	1.00 26.77	В
20	MOTA	4443	0	THR	248	9.168	9.077	33.914	1.00 27.38	В
	MOTA	4444	N	THR	249		8.732	35.092	1.00 26.76	В
	MOTA	4445	CA	THR	249	6.877	7.580	34.302	1.00 26.72	В,
	MOTA	4446	CB	THR	249	5.759	6.784	35.011	1.00 26.45	В
25	MOTA MOTA	4447	OG1		249 249	4.575	7.587 6.404	35.088	1.00 27.92	В
25	MOTA	4448 4449	CGZ	THR	249	6.180 6.353	8.040	36.423 32.938	1.00 25.26 1.00 27.55	В
	ATOM	4450	ò	THR	249	6.316	9.226	32.638	1.00 27.35	B B
	MOTA	4451	N	ILE	250	5.956	7.078	32.113	1.00 27.20	В
	MOTA	4452	CA	ILE	250	5.434	7.353	30.774	1.00 30.16	В
30	MOTA	4453	СВ	ILE	250	5.444	6.074	29.901	1.00 29.03	В
	MOTA	4454	CG2	ILE	250	4.410	5.082	30.421	1.00 27.86	B
	MOTA	4455	CG1	ILE	250	5.157	6.431	28.443	1.00 28.33	В
	MOTA	4456	CD1	ILE	250	5.425	5.295	27.476	1.00 26.91	В
25.	MOTA	4457	С	ILE	250	4.005	7.884	30.877	1.00 31.97	В
35	MOTA	4458	0	ILE	250	3.400	8.286	29.891	1.00 31.50	В
	MOTA	4459	N	ASP	251	3.477	7.875	32.095	1.00 34.02	В
	MOTA	4460	CA	ASP	251	2.132	8.368	32.359	1.00 36.26	В
	MOTA	4461	CB	ASP	251	1.425		33.381	1.00 36.12	В
40	MOTA MOTA	4462 4463	CG	ASP ASP	251 251	0.789 · 0.223	6.242 5.420	32.750	1.00 36.40	В
70	ATOM	4464		ASP	251	0.223	6.119	33.509 31.504	1.00 34.19	В
	ATOM	4465	C	ASP	251	2.164	9.804	32.910	1.00 36.03	8 B
	ATOM	4466	ō	ASP	251	1.140	10.468	32.990	1.00 38.11	В
	ATOM	4467	N	GLY	252	3.350	10.273	33.284	1.00 37.77	В
45	MOTA	4468	CA	GLY	252	3.471	11.613	33.822	1.00 37.41	В
	MOTA	4469	С	GLY	252	3.566	11.662	35.338	1.00 38.71	В
	MOTA	4470	Ο.	GLY	252	3.747	12.734	35.912	1.00 38.78	В
	MOTA	4471	N	GLU	253	3.440	10.516	36.003	1.00 38.85	В
50	MOTA	4472	CA	GLU	253	3.533	10.511	37.459	1.00 39.67	В
50	MOTA	4473	CB	GLU	253	3.020	9.200	38.052	1.00 41.37	В
	MOTA MOTA	4474 4475	CD	GLU	253 253	3.181 2.814	9.143 7.803	39.573	1.00 43.75	В
	ATOM	4476		GLU	253	3.083	7.612	40.188 41.398	1.00 44.31	B B
	ATOM	4477		GLU	253	2.256	6.945	39.470	1.00 45.10	В
55	ATOM	4478	Ċ	GLU	253	4.988	10.668	37.883	1.00 39.49	В
	ATOM	4479	0	GLU	253	5.890	10.286	37.149	1.00 39.20	В
	ATOM	4480	N	GLU	254		11.239	39.064	1.00 39.27	В
	MOTA	4481	CA	GLU	254	6.568	11.426	39.567	1.00 40.50	В.
۲۵	ATOM	4482	CB	GLU	254	6.793	12.875	39.978	1.00 41.13	В
60	MOTA	4483	CG	GLU	254	6.621	13.842	38.836	1.00 44.09	В
	ATOM	4484	CD	GLU	254	7.073	15.233	39.189	1.00 45.25	В
	MOTA	4485		GLU	254	6.665	15.737	40.256	1.00 45.35	В
	MOTA	4486		GLU	254	7.828	15.825	38.391	1.00 46.38	В
65	ATOM ATOM	4487 4488	0	GLU	254 254	6.926	10.539	40.756	1.00 39.50	В
-	ATOM	4489	Ŋ	GLU LEU	255	6.242 8.008	10.540	41.769	1.00 40.75 1.00 37.82	В
	ATOM	4490	CA	LEU	255 255	8.484	9.779 8.894	40.614 41.676	1.00 37.82	В
	ATOM	4491	CB	LEU	255 255	8.895	7.543	41.076	1.00 35.11	B B
	ATOM	4492	CG	LEU	255	7.950	6.910	40.062	1.00 35.67	В
70	ATOM	4493		LEU	255	8.538	5.614	39.590	1.00 35.24	В
	MOTA	4494		LEU	255	6.601	6.663	40.668	1.00 35.26	. В
	MOTA	4495	С.	LEU	255	9.710	9.551	42.322	1.00 35.19	В
	MOTA	4496	0	LEU	255	10.722	9.754	41.644	1.00 35.09	В

	ATOM	4497	N	VAL	256	9.612	9.888	43.615	1.00 33.29	В
	ATOM	4498	CA	VAL	256	10.719	10.528	44.350	1.00 31.53	В
	ATOM	4499	CB	VAL	256	10.237	11.748	45.143	1.00 31.44	В
	ATOM	4500	CG1	VAL	256	9.719	12.800	44.188	1.00 30.73	В
5	ATOM	4501	CG2		256	9.165	11.322	46.141	1.00 33.02	В
•	MOTA	4502	C	VAL	256	11.494	9.622	45.319	1.00 29.50	В
	MOTA	4503			256	10.928				
			0	VAL			8.958	46.189	1.00 29.05	В
	ATOM	4504	N	LYS	257	12.809	9.604	45.148	1.00 27.07	В
10	MOTA	4505	CA	LYS	257	13.676	8.790	45.985	1.00 24.38	В
10	MOTA	4506	CB	LYS	257	14.530	7.832	45.134	1.00 21.73	В
	MOTA	4507	CG	LYS	257	13.742	6.776	44.369	1.00 18.70	В
	MOTA	4508	CD	LYS	257	14.637	5.862	43.566	1.00 13.96	В
	ATOM	4509	CE	LYS	257	15.316	6.632	42.460	1.00 12.43	В
	MOTA	4510	NZ	LYS	257	16.093	5.743	41.576	1.00 10.28	В
15	ATOM	4511	Č	LYS		14.627	9.701		1.00 10.28	
1.0					257			46.731		В
	MOTA	4512	0	LYS	257	15.062	10.708	46.215	1.00 24.31	В
	MOTA		. N	ILE	258	14.928	9.357	47.970	1.00 22.97	В
	MOTA	4514	CA	ILE	258	15.882	10.138	48.741	1.00 20.65	В
00	MOTA	4515	CB	ILE	258	15.226	10.866	49.913	1.00 22.22	В
20	MOTA	4516	CG2	ILE	258	16.246	11.747	50.591	1.00 22.81	В
	MOTA	4517	CG1	ILE	258	14.080	11.734	49.407	1.00 24.53	В
	ATOM .	4518	CD1	ILE	258	13.276	12.417	50.518	1.00 24.98	В
	ATOM	4519	c	ILE	258	16.891	9.136	49.271	1.00 18.47	В
	ATOM	4520	ŏ	ILE	258	16.554	8.243	50.049	1.00 16.24	В
25	MOTA	4521	N	GLY	259	18.123	9.256	48.805		В
23									1.00 17.79	
	MOTA	4522	CA	GLY	259	19.144	8.342	49.262	1.00 18.70	. В
	ATOM	4523		GLY	. 259	20.205	9.094	50.030	1.00 17.80	В
	ATOM	4524	0	GLY	259	20.684	10.110	49.555	1.00 18.70	В
20	MOTA	4525	N	LYS	260	20.565	8.606	51.215	1.00 16.12	В
30	MOTA	4526	CA	LYS	260	21.598	9.263	52.011	1.00 15.58	В
	ATOM	4527	CB	LYS	260	21.034	9.800	53.335	1.00 15.55	В
	MOTA	4528	CG	LYS	260	21.889	10.844	54.046	1.00 14.21	В
	MOTA	4529	CD	LYS	260.	21.173	11.288	55.341	1.00 15.40	B
	ATOM	4530	CE	LYS	260	21.989	12.289	56.170	1.00 13.76	В
35	MOTA	4531	NZ	LYS	260	21.311	12.687	57.451		
55										В
	ATOM	4532	C	LYS	260	22.729	8.309	52.335	1.00 13.87	В
	MOTA	4533	0	LYS	260	22.531	7.185	52.741	1.00 13.84	В
	MOTA	4534	N	LEU	261	23.937	8.788	52.141	1.00 13.07	В
in	MOTA	4535	CA	LEU	261	25.107	7.996	52.430	1.00 11.82	В
40	MOTA	4536	CB	LEU	261	25.890	7.772	51.130	1.00 10.77	B
	MOTA	4537	CG	LEU	261	27.276	7.138	51.238	1.00 8.89	В
	MOTA	4538	CD1	LEU	261	27.189	5.799	51.975	1.00 7.84	В
	MOTA	4539		LEU	261	27.847	6.973	49.840	1.00 7.48	В
	MOTA	4540	c	LEU	261	25.993	8.696	53.465	1.00 11.44	В
45	ATOM	4541	ŏ	LEU	261	26.424	9.819	53.247	1.00 13.74	
7.5		4542								В
	ATOM		N	ASN	262	26.245	8.024	54.586	1.00 10.57	В
	ATOM	4543	CA	ASN	262	27.142	8.548	55.615	1.00 8.04	В
	MOTA	4544	CB	ASN	262	26.494	8.386	56.985	1.00 5.60	В
50	ATOM	4545	CG	ASN	262	25.111	8.980	57.011	1.00 8.99	В
50	ATOM	4546	OD1	ASN	262	24.100	8.263	56.971	1.00 9.21	В
	ATOM	4547	ND2	ASN	262	25.050	10.307	57.024	1.00 7.62	В
	ATOM	4548	С	ASN	262	28.526	7.879	55.554	1.00 6.87	В
	MOTA	4549	0	ASN	262	28.640	6.653	55.523	1.00 7.74	В
	ATOM	4550	N	LEU	263	29.566	8.705	55.487	1.00 5.79	В
55	ATOM	4551	CA	LEU	263	30.938	8.225	55.438	1.00 5.65	В
55	ATOM	4552	CB	LEU	263	31.596	8.741	54.165		
									1.00 4.90	В
	ATOM	4553	CG	LEU	263	30.735	8.279	52.998	1.00 6.08	В
	MOTA	4554	CD1		263	31.131	9.012	51.752	1.00 5.33	В
<i>c</i>	MOTA	4555		LEU	263	30.853	6.748	52.877	1.00 6.04	В
60	ATOM	4556	С	LEU	263	31.634	8.694	56.710	1.00 6.26	В
	ATOM	4557	0	LEU	263	32.017	9.853	56.842	1.00 8.01	В
	ATOM	4558	N	VAL	264	31.795	7.778	57.653	1.00 6.21	В
	MOTA	4559	CA	VAL	264	32.406	8.079	58.943	1.00 6.25	В
	ATOM	4560	CB	VAL	264	31.600	7.410	60.037	1.00 7.30	В
65	MOTA	4561	CG1		264	32.081	7.848	61.406	1.00 6.21	В
-	MOTA	4562	CG2		264	30.140	7.709			
	MOTA							59.802	1.00 9.51	В
		4563	Ç	VAL	264	33.863	7.677	59.150	1.00 7.28	В
	ATOM	4564	0	VAL	264	34.221	6.532	58.978	1.00 7.31	В
70	MOTA	4565	N	ASP	265	34.685	8.652	59.533	1.00 9.79	В
70	MOTA	4566	CA	ASP	265	36.105	8.441	59.841	1.00 11.34	В
	ATOM	4567	CB	ASP	265	36.978	9.564	59.262	1.00 12.62	В
	ATOM	4568	CG	ASP	265	38.473	9.346	59.520	1.00 16.17	В
	ATOM	4569	OD1		265	38.801	8.748	60.562	1.00 17.08	В
									- · · - ·	

	ATOM	4570	OD2	ASP	265	39.310	9.783	58.694	1.00 16.43	В
	MOTA	4571	С	ASP	265	36.179	8.527	61.374	1.00 11.75	В
	MOTA	4572	0	ASP	265	36.356	9.601	61.928	1.00 11.74	В
_	ATOM	4573	N	LEU	266	36.032	7.389	62.051	1.00 12.21	В
5	MOTA	4574	CA	LEU	266	36.054	7.367	63.519	1.00 13.54	В
	ATOM	4575	СВ	LEU	266	35.692	5.986	64.068	1.00 13.06	В
	MOTA	4576	CG	LEU	266	34.327	5.426	63.711	1.00 14.69	В
	MOTA	4577	CD1	LEU	266	34.190	3.979	64.232	1.00 13.37	В
	ATOM	4578	CD2	LEU	266	33.266	6.350	64.285	1.00 14.29	В
10							7.763			
10	MOTA	4579	C	LEU	266	37.366		64.193	1.00 14.66	В
	MOTA	4580	0	LEU	266	38.437	7.776	63.580	1.00 16.77	. В
	ATOM	4581	N	ALA	267	37.267	8.097	65.474	1.00 15.57	В
	ATOM	4582	CA	ALA	267	38.435	8.494	66.237	1.00 15.49	B
1.5	MOTA	4583	CB	ALA	267	38.015	9.063	67.584	1.00 15.66	В
15	MOTA	4584	С	ALA	267 .	39.281	7.256	66.427	1.00 16.90	В
	ATOM	4585	0	ALA	267	38.752	6.166	66.492	1.00 17.09	В
	MOTA	4586	N	GLY	268	40.594	7.432	66.535	1.00 18.45	. В
	MOTA	4587	CA	GLY	268	41.470	6.286	66.684	1.00 19.06	В
	MOTA	4588	С	GLY	268	40.979	5.375	67.779	1.00 20.29	В
20	MOTA	4589	0	GLY	268	40.476	5.846	68.778	1.00 22.63	В
	ATOM	4590	N	SER	269	41.153	4.070	67.608	1.00 21.30	В
	ATOM .	4591	CA	SER	269	40.683	3.127	68.611	1.00 21.55	В
	MOTA	4592	CB	SER	269	40.151	1.869	67.940	1.00 19.85	В
	MOTA	4593	OG	SER	269	41.174	1.230	67.206	1.00 19.77	В
25	ATOM	4594	C	SER	269	41.696	2.703	69.666	1.00 23.07	· B
	MOTA	4595	0	SER	269	41.415	1.832	70.461	1.00 23.77	. В
	MOTA	4596	N	.GLU	270	42.863	3.336	69.682	1.00 24.72	В
	MOTA	4597	CA	GLU	270	43.889	2.997	70.666	1.00 26.45	B
	ATOM	4598	CB	GLU	270	45.255	3.538	70.212	1.00 26.88	В
30	ATOM	4599	CG	GLU	270	45.365	5.074	70.179	1.00 26.65	В
50										
	MOTA	4600	CD	GLU	270	44.769	5.716	68.938	1.00 25.63	В
	ATOM	4601	OE1	GLU	270	44.782	6.966	68.848	1.00 25.90	В
	ATOM	4602	OE2	GLU	270.	44.299	4.966	68.063	1.00 25.37	В
	MOTA	4603	С	GLU	270	43.595	3.501	72.096	1.00 28.21	В
35	ATOM	4604	ō	GLU	270		4.646	72.317		
55						43.182			1.00 27.82	В -
	MOTA	4605	N	ASN	271	43.804	2.619	73.066	1.00 31.11	В
	· ATOM	4606	CA	ASN	271	43.590	2.932	74.483	1.00 33.53	В
	ATOM	4607	CB	ASN	. 271	42.239	3.620	74.720	1.00 35.28	В
	ATOM	4608	CG	ASN	271	41.046	2.755	74.319	1.00 37.15	B
40										
40	MOTA	4609		ASN	271	39.892	3.159	74.481	1.00 37.89	В
	MOTA	4610	NDZ	ASN	271	41.319	1.569	73.789	1.00 38.13	В
	ATOM	4611	С	ASN	271	43.617	1.669	75.326	1.00 34.61	В
	ATOM	4612	0	ASN	271	43.637	0.561	74.789	1.00 35.03	В
	ATOM	4613	N	ASN	287	41.713	11.898	79.742	1.00 41.72	В
45										
43	MOTA	4614	CA	ASN	287	40.726	12.291	78.737	1.00 42.10	В
	ATOM	4615	CB	ASN	. 287	41.389	13.166	77.666	1.00 43.36	В
	ATOM	4616	CG	ASN	287	42.137	14.334	78.263	1.00 44.01	В
	MOTA	4617		ASN	287	43.107	14.144	78.990	1.00 44.40	В
	ATOM	4618		ASN	287		15.548	77.967		
50						41.688			1.00 44.56	В
20	MOTA	4619	С	ASN	287	40.094	11.054	78.083	1.00 41.01	В
	MOTA	4620	0	ASN	287	40.802	10.130	77.661	1.00 42.34	В
	MOTA	4621	N	ILE	288	38.764	11.039	77.994	1.00 37.53	В
	MOTA	4622	CA	ILE	288	38.053	9.905	77.397	1.00 33.20	В
	ATOM	4623	CB	ILE	288	37.119	9.256	78.433		
55									1.00 33.55	В
22	MOTA	4624		ILE	288	37.940	8.681	79.575	1.00 32.67	В
	MOTA	4625	CG1	ILE	288	36.142	10.308	78.967	1.00 33.79	В
	MOTA	4626	CD1	ILE	288	35.028	9.764	79.828	1.00 33.58	В
	MOTA	4627	С	ILE	288	37.221	10.255	76.147	1.00 29.09	В
	MOTA	4628	ŏ	ILE	288	36.810	11.410	75.946		
60									1.00 28.30	В
UU	MOTA	4629	N	ASN	289	36.975	9.258	75.303	1.00 23.27	В
	MOTA	4630	CA	ASN	289	36.172	9.492	74.116	1.00 19.88	В
	MOTA	4631	CB	ASN	289	36.898	8.993	72.871	1.00 18.84	В
	MOTA	4632	CG	ASN	289	36.379	9.622	71.601	1.00 19.35	В
	ATOM	4633		ASN	289	37.155	10.094		1.00 21.16	
65								70.786		В
UJ.	MOTA	4634	ND2		289	35.065	9.612	71.415	1.00 18.98	В
	ATOM	4635	С	ASN -	289	34.829	8.805	74.326	1.00 18.28	В
	MOTA	4636	0	ASN	289	34.628	7.609	74.013	1.00 16.89	В
	MOTA	4637	N	GLN	290	33.906	9.579	74.884	1.00 16.97	В
	ATOM	4638	CA		290	32.560	9.115		1.00 14.08	
70				CLN				75.178		В
70	MOTA	4639	CB	GLN	290	31.741	10.277	75.738	1.00 15.20	В
	MOTA	4640	CG	GLN	290	30.328	9.905	76.161	1.00 16.32	В
	MOTA	4641	CD	GLN	290	30.274	8.855	77.266	1.00 16.30	В
	ATOM	4642		GLN	290	29.232	8.273	77.512	1.00 16.57	В
					-					_

	ATOM	4643	NE2	GLN	290	31.401	8.621	77.934	1.00 17.40	В
	ATOM	4644	C	GLN	. 290	31.856	8.520	73.959	1.00 12.46	В
	MOTA	4645	0	GLN	290	31.207	7.500	74.055	1.00 12.26	В
_	MOTA	4646	N	SER	291	31.971	9.174	72.814	1.00 11.04	В
5	MOTA	4647	CA	SER	291	31.333	8.627	71.629	1.00 11.96	В
	ATOM	4648	CB	SER	291	31.404	9.609	70.466	1.00 11.35	В
	MOTA	4649	OG	SER	291	30.393	10.586	70.582	1.00 12.37	В
	MOTA	4650	С	SER	291	31.950	7.299	71.201	1.00 11.18	В
	ATOM	4651	0	SER	291	31.241	6.375	70.783	1.00 11.32	В
10	ATOM	4652	Ň	LEU	292	33.270	7.205	71.294	1.00 11.69	B
10										
	MOTA	4653	CA	LEU	292	33.965	5.984	70.919	1.00 11.36	В
	MOTA	4654	CB	LEU	292	35.485	6.237	70.902	1.00 9.67	В
	MOTA	4655	CG	LEU	292	36.263	5.054	70.334	1.00 10.97	В
	MOTA	4656		LEU	292	35.817	4.822	68.911	1.00 10.21	В
. 15	ATOM				292	37.750	5.328	70.387		В
13		4657		LEU					1.00 13.35	
	MOTA	4658	С	LEU	292	33.574	4.877	71.914	1.00 11.82	В
	ATOM	4659	0	LEU	292	33.287	3.724	71.527	1.00 11.11	В
	MOTA	4660	N	LEU	293	33.547	5.232	73.194	1.00 8.02	В
	ATOM	4661	CA	LEU	293	33.210	4.295	74.246	1.00 7.35	В
20										
20	MOTA	4662	CB	LEU	293	33.313	5.005	75.596	1.00 5.38	В
	MOTA	4663	CG	LEU	293	34.410	4.587	76.570	1.00 6.04	В
	MOTA	4664	CD1	LEU	293	35.605	3.981	75.841	1.00 3.22	В
	ATOM	4665		LEU	293	34.798	5.808	77.389	1.00 3.25	В
25	MOTA	4666	С	LEU	293	31.802	3.747	74.071	1.00 7.33	·B
25	MOTA	4667	0	LEU	293	31.563	2.550	74.222	1.00 9.04	В
	MOTA	4668	N	THR	294	30.874	4.646	73.775	1.00 8.36	В
	ATOM	4669	CA	THR	294	29.481	4.283	73.604	1.00 6.48	В
	ATOM	4670	CB	THR	294	28.623	5.535	73.600		
									1.00 5.81	В
20	MOTA	4671		THR	294	28.889	6.251	74.804	1.00 6.32	В
30	MOTA	4672	CG2	THR	294	27.142	5.206	73.570	1.00 4.45	В
	ATOM	4673	С	THR	294	29.237	3.461	72.364	1.00 7.94	В
	ATOM	4674	ō	THR	294	28.357	2.602	72.368	1.00 9.76	В
	MOTA	4675	N	LEU	295	30.016	3.706	71.310	1.00 6.67	В
0.5	MOTA	4676	CA	LEU	295	29.896	2.918	70.074	1.00 6.68	В
35 ⁻	ATOM	4677	CB	LEU	295	30.931	3.313	69.016	1.00 6.59	В
	MOTA	4678	CG	LEU	295	30.897	2.510	67.708	1.00 5.44	В
	MOTA	4679		LEU	295	29.555	2.668	67.036	1.00 4.15	
										В
	MOTA	4680	CD2	LEU	295	31.969	2.993	66.786	1.00 5.26	В
	MOTA	4681	С	LEU	295	30.228	1.473	70.403	1.00 8.24	В
40	MOTA	4682	0	LEU	295	29.615	0.555	69.887	1.00 9.80	В
. •	MOTA	4683	N	GLY	296	31.214	1.290	71.276	1.00 9.60	В
	MOTA	4684	CA	GLY	296	31.611	~0.047	71.669	1.00 10.99	В
	MOTA	4685	С	GLY	296	30.551	-0.728	72.518	1.00 12.56	В
	MOTA	4686	0	GLY	296	30.275	-1.924	72.350	1.00 12.84	В
45	MOTA	4687	N	ARG	297	29.954	0.037	73.426	1.00 12.22	В
	ATOM	4688	CA	ARG	297	28.928	-0.486	74.307		
									1.00 12.41	В
	MOTA	4689	CB	ARG	297	28.692	0.466	75.478	1.00 11.73	В
	MOTA	4690	CG	ARG	297	29.818	0.493	76.498	1.00 10.69	В
	MOTA	4691	CD	ARG	297	29.767	1.736	77.378	1.00 11.84	В
50	MOTA	4692	NE	ARG	297	30.969	1.856	78.205	1.00 10.74	В
		4693	cz	ARG				_		
	MOTA				297	31.409	2.993	78.734	1.00 10.49	В
	MOTA	4694	NH1		297	30.743	4.119	78.517	1.00 11.64	В
	ATOM	4695	NH2	ARG	297	32.504	3.003	79.486	1.00 9.73	В
	ATOM	4696	С	ARG	297	27.622	-0.708	73.569	1.00 13.86	В
55	ATOM	4697	ō	ARG	297	26.798	-1.514	74.009	1.00 13.06	В
55										
	MOTA	4698	N	VAL	298	27.426	0.014	72.464	1.00 14.33	В
	MOTA	4699	CA	VAL	298	26.216	-0.134	71.659	1.00 16.21	В
	ATOM	4700	CB	VAL	298	26.048	1.031	70.696	1.00 16.05	В
	ATOM	4701	CG1		298	25.021	0.679	69.639	1.00 17.88	В
60										
00	MOTA	4702	CG2		298	25.605	2.257	71.458	1.00 18.13	B
	MOTA	4703	С	VAL	298	26.281	-1.426	70.853	1.00 17.16	В
	MOTA	4704	0	VAL	298	25.305	-2.173	70.774	1.00 18.74	В
	ATOM	4705	N	ILE	299	27.441	-1.691	70.262	1.00 18.24	В
65	MOTA	4706	CA	ILE	299	27.645	-2.910	69.486	1.00 18.96	В
65	MOTA	4707	CB	ILE	299	29.019	-2.868	68.770	1.00 19.68	В
	ATOM	4708	CG2	ILE	299	29.368	-4.245	68.184	1.00 17.64	В
	MOTA	4709		ILE	299	28.983	-1.791	67.674	1.00 19.70	В
	MOTA	4710		ILE	299	30.314	-1.589	66.977	1.00 22.74	
										В
70	ATOM	4711	c	ILE	299	27.551	-4.142	70.400	1.00 19.56	В
70	MOTA	4712	0	ILE	299	27.027	-5.191	70.012	1.00 19.03	В
	ATOM	4713	N	THR	300	28.043	-4.017	71.624	1.00 19.86	В
	MOTA	4714	CA	THR	300	27.978	-5.136	72.551	1.00 20.92	В
	ATOM	4715	CB	THR	300	28.770	-4.841	73.824	1.00 20.58	В

	ATOM	4716	001	THR	300	30.172	-4.893	73.533	1.00 21.97	
										В
	MOTA	4717	CG2	THR	300	28.433	-5.845	74.903	1.00 21.65	В
	MOTA	4718	С	THR	300	26.525	-5.450	72.915	1.00 21.71	В
_	MOTA	4719	0	THR	300	26.134	-6.601	72.984	1.00 22.71	В
5	ATOM	4720	N	ALA	301	25.728	-4.413	73.139	1.00 23.13	В
_										
	ATOM	4721	CA	ALA	301	24.337	-4.624	73.494	1.00 23.01	В
	MOTA	4722	CB	ALA	301	23.694	-3.327	73.904	1.00 22.73	В
				ALA	301	23.589	-5.225	72.323	1.00 23.48	
	MOTA	4723	С							В
	ATOM	4724	0	ALA	301	22.652	-5.982	72.509	1.00 23.63	В
10	ATOM	4725	N	LEU	302	24.005	-4.872	71.111	1.00 23.21	В
10										
	MOTA	4726	CA	LEU	302	23.361	-5.392	69.911	1.00 24.59	В
	ATOM	4727	CB	LEU	302	23.737	-4.526	68.695	1.00 23.93	В
	MOTA	4728	CG	LEU	302	22.774	-3.511	68.059	1.00 22.99	В
	ATOM	4729	CD1	LEU	302	21.827	-2.952	69.058	1.00 20.71	В
15	ATOM	4730		LEU	302	23.579	-2.394	67.440	1.00 21.49	В
13										
	MOTA	4731	С	LEU	302	23.728	-6.861	69.656	1.00 25.70	В
	ATOM	4732	. 0	LEU	302	22.847	-7.695	69.406	1.00 24.83	В
	MOTA	4733	N	VAL	303	25.021	-7.170	69.731	1.00 27.74	В
	MOTA	4734	CA	VAL	303	25.527	-8.521	69.505	1.00 29.35	. в
20										
20	MOTA	4735	CB	VAL	303	27.054	-8.549	69.593	1.00 29.55	В
	MOTA	4736	CG1	VAL	303	27.545	-9.975	69.439	1.00 30.49	В
	ATOM	4737	CG2	VAL	303	27.651	-7.641	68.524	1.00 30.24	В
	MOTA	4738	С	VAL	303	24.985	-9.528	70.510	1.00 31.00	В
	MOTA	4739	0	VAL	303	24.629	-10.631	70.160	1.00 30.43	В
25										
23	ATOM	4740	N	GLU	304	24.927	-9.123	71.770	1.00 33.86	В
	MOTA	4741	CA	GLU	304	24.442	-9.986	72.838	1.00 36.40	. в
		4742								
	ATOM			GLU	304	25.130	-9.594	74.143	1.00 37.33	В
	ATOM	4743	CG	GLU	304	26.650	-9.690	74.076	1.00 39.18	В
	ATOM	4744	CD	GLU	304	27.316	-9.437	75.422	1.00 41.19	В
30										
JU	MOTA	4745	OE1	GLU	304	28.564	-9.473	75.490	1.00 42.27	В
	ATOM	4746	OE2	GLU	304	26.594	-9.202	76.413	1.00 42.10	В
	MOTA	4747	С	GLU	304	22.922	-9.924	72.985	1.00 38.11	В
	ATOM	4748	0	GLU	304	22.334	-10.552	73.871	1.00 37.60	В
	ATOM		N	ARG	305	22.303	-9.155	72.098	1.00 41.03	
25		4749								В
35	MOTA	4750	CA	ARG	305	20.860	-8.996	72.068	1.00 43.26	В
	ATOM	4751	CB	ARG	305		-10.302	71.592	1.00 44.67	В
	ATOM	4752	CG	ARG	305	20.602	-10.629	70.151	1.00 46.86	В
	MOTA	4753	CD	ARG	305	20.167	-12.025	69.716	1.00 49.68	В
40	MOTA	4754	NE	ARG	305	20.654	-12.350	68.373	1.00 50.79	B
40	ATOM	4755	cz	ARG	305	20.244	-11.753	67.258	1.00 50.97	В
_	ATOM	4756		ARG	305		-10.797	67.309		В
									1.00 51.47	
	ATOM	4757	NH2	ARG	305	20.769	-12.097	66.089	1.00 51.54	В
	MOTA	4758	С	ARG	305	20.237	-8.514	73.367	1.00 43.49	В
4 ~	MOTA	4759	0	ARG	305	19.142	-8.909	73.718	1.00 44.11	В
45	MOTA	4760	N	THR	306	20.951	-7.648	74.077	1.00 44.17	В
	ATOM	4761	CA	THR	306	20.444	-7.078	75.319	1.00 43.76	В
	MOTA	4762	CB	THR	306	21.535	-6.267	76.040	1.00 43.72	В
	MOTA	4763	OG1	THR	306	22.623	-7.131	76.399	1.00 43.84	В
~~	ATOM	4764	CG2	THR	306	20.975	-5.602	77.288	1.00 43.30	В
50	ATOM	4765	С	THR	306	19.307	-6.139	74.912	1.00 44.17	В
	MOTA	4766	0	THR	306	19.388	-5.459	73.891	1.00 45.09	
										В
	MOTA	4767	N	PRO	307	18.226	-6.098	75.700	1.00 43.54	В
	MOTA	4768	CD	PRO	307	17.925	-6.973	76.846	1.00 43.66	В
e e	MOTA	4769	CA	PRO	307	17.080	-5.232	75.390	1.00 42.75	В
55	MOTA	4770	CB	PRO	307	16.101	-5.554	76.518	1.00 43.35	В
	ATOM	4771	CG	PRO	307	16.429	-7.001	76.834	1.00 44.16	В
	MOTA	4772	Ç	PRO	307	17.408	-3.741	75.269	1.00 41.65	В
	MOTA	4773	0	PRO	307	16.903	-3.049	74.384	1.00 41.15	В
~ ^	MOTA	4774	N	HIS	308	18.254	-3.247	76.166	1.00 39.72	В
60	MOTA	4775	CA	HIS	308	18.629	-1.839	76.164	1.00 37.51	В
	ATOM	4776	CB	HIS	308	18.774	-1.336	77.587	1.00 39.81	
										В
	MOTA	4777	CG	HIS	308	19.193	0.097	77.677	1.00 42.26	В
	MOTA	4778	CD2		308	20.336	0.664	78.127	1.00 43.26	В
	MOTA	4779	ND1		308	18.391	1.131	77.247	1.00 43.54	В
65	ATOM	4780	CE1	HIS	308	19.024	2.278	77.428	1.00 44.49	В
	ATOM	4781	NE2		308	20.205	2.024	77.959	1.00 44.29	В
	ATOM	4782	С	HIS	308	19.937	-1.559	75.446	1.00 35.63	В
	MOTA	4783	0	HIS	308	20.958	-2.160	75.745	1.00 36.69	В
70	ATOM	4784	N	VAL	309	19.889	-0.627	74.501	1.00 32.04	В
70	MOTA	4785	CA	VAL	309	21.071	-0.237	73.731	1.00 27.44	В
-										
	ATOM	4786	CB	VAL	309	20.821	-0.415	72.218	1.00 27.23	В
	ATOM	4787	CG1	VAL	309	22.090	-0.111	71.426	1.00 27.83	В
	ATOM	4788	CG2		309	20.336	-1.823	71.946	1.00 25.00	В
							2.023		23.00	U

	ATOM	4789	C	VAL	309	21.307	1:234	74.059	1.00 26.45	. В
	ATOM	4790	ŏ	VAL	309	20.501	2.090	73.724	1.00 26.41	В
	MOTA	4791	N	PRO	310	22.432	1.538	74.715	1.00 25.12	
										В
5	MOTA	4792	CD	PRO	310	23.508	0.587	75.062	1.00 23.57	B
5	MOTA	4793	CA	PRO	310	22.780	2.914	75.107	1.00 22.73	В
	MOTA	4794	СВ	PRO	310	23.985	2.701	76.007	1.00 23.56	В
	ATOM	4795	CG	PRO	310	24.671	1.504	75.354	1.00 23.96	В
	MOTA	4796	С	PRO	310	23.017	3.958	73.999	1.00 22.22	В
10	MOTA	4797	0	PRO	310	23.965	4.735	74.073	1.00 21.14	В
10	MOTA	4798	N	TYR	311	22.147	4.000	72.995	1.00 21.70	В
	MOTA	4799	·CA	TYR	311	22.294	4.967	71.899	1.00 22.33	В
	MOTA	4800	CB	TYR	311	21.083	4.978	70.970	1.00 22.30	В
	ATOM	4801	CG	TYR	311	20.861	3.721	70.154	1.00 24.68	В
	ATOM	4802		TYR	311	21.773	3.322	69.177	1.00 25.08	B
15	ATOM	4803		TYR	311	21.555	2.171	68.411	1.00 25.18	В
	ATOM	4804		TYR	311	19.717	2.937	70.347	1.00 24.09	B
	ATOM	4805		TYR	311	19.493	1.786	69.590	1.00 24.09	В
	MOTA	4806	CZ	TYR	311	20.416	1.405	68.623	1.00 24.98	В
	ATOM	4807	OH	TYR	311	20.211	0.246	67.893	1.00 24.66	В
20	MOTA	4808		TYR				72.338		
20			Ç		311	22.431	6.429		1.00 21.98	В
	MOTA	4809	0	TYR	311	23.180	7.188	71.741	1.00 23.57	В
	MOTA	4810	N	ARG	312	21.707	6.813	73.384	1.00 20.49	В.
	MOTA	4811	CA	ARG	312	21.726	8.203	73.861	1.00 19.38	В
25	MOTA	4812	CB	arg	312	20.447	8.544	74.640	1.00 21.56	·B
25	MOTA	4813	CG	ARG	312	19.150	8.149	73.951	1.00 24.98	В
	MOTA	4814	CD	ARG	312	17.949	8.887	74.534	1.00 27.94	В
	MOTA	4815	NE	ARG	312	16.688	B.240	74.175	1.00 31.63	В
	MOTA	4816	CZ	ARG	312	16.262	7.086	74.688	1.00 34.10	В
~~	MOTA	4817	NH1	ARG	312	16.996	6.445	75.590	1.00 37.15	· в
30	MOTA	4818	NH2	ARG	312	15.101	6.566	74.304	1.00 33.60	В
	MOTA	4819	С	ARG	312	22.875	8.612	74.779	1.00 17.27	В
	MOTA	4820	0	ARG	312	22.933	9.756	75.235	1.00 16.64	В
	ATOM	4821	N	GLU	313	23.786	7.686	75.054	1.00 14.25	В
	MOTA	4822	CA	GLU	313	24.908	7.986	75.935	1.00 11.55	В
35 [°]	ATOM '	4823	CB	GLU	313	25.410	6.693	76.590	1.00 11.14	В
	ATOM	4824	CG	GLU	313	24.416	6.136	77.618	1.00 11.41	В
	ATOM	4825	CD	GLU	313	24.916	4.905	78.379	1.00 12.57	В
	ATOM	4826		GLU			4.898	78.834	1.00 12.37	
	ATOM	4827		GLU						В
40	ATOM				313	24.149	3.935	78.569	1.00 14.80	В
70		4828	C	GLU	313	26.053	8.746	75.271	1.00 10.23	В
	MOTA	4829	0	GLU	313	27.066	8.960	75.891	1.00 10.15	В
	MOTA.	4830	N	SER	314	25.865	9.164	74.017	1.00 10.36	В
	ATOM	4831	CA	SER	314	26.878	9.912	73.263	1.00 9.41	В
15	MOTA	4832	CB	SER	314	28.000	9.018	72.732	1.00 10.81	В
45	MOTA	4833	OG	SER	314	27.643	8.320	71.544	1.00 9.64	В
	MOTA	4834	Ç	SER	314	26.235	10.511	72.031	1.00 10.05	В
	MOTA	4835	Ο.	SER	314	25.190	10.052	71.583	1.00 9.18	В
	MOTA	4836	N	LYS	315	26.887	11.544	71.501	1.00 10.81	В
~~	ATOM	4837	CA	LYS	315	26.428	12.259	70.320	1.00 9.07	В
50	ATOM	4838	CB	LYS	315	27.254	13.527	70.063	1.00 9.50	В
	MOTA	4839	CG	LYS	315	27.390	14.463	71.236	1.00 9.25	В
	ATOM	4840	CD	LYS	315 .	26.058	14.973	71.686	1.00 10.89	В
	MOTA	4841	CE	LY\$	315	26.244	16.156	72.620	1.00 13.02	В
	ATOM	4842	NZ	LYS	315	26.918	17.316	71.937	1.00 14.10	В
55	MOTA	4843	С	LYS	315	26.556	11.414	69.077	1.00 8.68	В
	MOTA	4844	ō	LYS	315	25.652	11.383	68.282	1.00 10.14	В
	ATOM	4845	Ň	LEU	316	27.683	10.721	68.931	1.00 8.28	_
	ATOM	4846	CA	LEU	316	27.928	9.888	67.763	1.00 7.48	B.
•	ATOM	4847	СВ	LEU	316	29.297	9.205	67.867	1.00 6.90	
60	ATOM	4848	CG		316		8.277			В
00				LEU		29.679		66.713	1.00 8.06	В
	ATOM	4849		LEU	316	30.018	9.097	65.484	1.00 10.24	В
	ATOM	4850		LEU	316	30.850	7.452	67.129	1.00 8.22	В
	ATOM	4851	С	LEU	316	26.852	8.821	.67.590	1.00 9.38	В
45	MOTA	4852	0	LEU	316	26.241	8.733	66.523	1.00 9.82	В
65	MOTA	4853	N	THR	317	26.588	8.040	68.642	1.00 9.80	В
	ATOM	4854	CA	THR	317	25.599	6.965	68.534	1.00 10.18	В
	MOTA	4855	CB	THR	317	25.672	5.952	69.674	1.00 10.15	В
	MOTA	4856	0G1	THR	317	25.527	6.642	70.909	1.00 10.81	В
	ATOM	4857	CG2	THR	317	27.004	5.185	69.661	1.00 9.59	В
70	MOTA	4858	C	THR	317	24.175	7.455	68.484	1.00 10.03	В
	ATOM	4859	Ö	THR	317	23.295	6.709	68.146	1.00 11.71	В
	ATOM	4860	N	ARG	318	23.947	8.703	68.867	1.00 9.69	В
	ATOM	4861	CA	ARG	318	22.607	9.256	68.785	1.00 9.04	B
									- -	_

	ATOM	4862	CB	ARG	318	22.454	10.464	69.703	1.00 13.23	В
	MOTA	4863	CG	ARG	318	21.719	10.147	71.004	1.00 19.08	В
	MOTA	4864	CD	ARG	318	22.058	11.133	72.115	1.00 22.73	В
	MOTA	4865	NE	ARG	318	21.617	12.495	71.828	1.00 26.31	В
5	MOTA							71.705		
,		4866	cz	ARG	318	. 20.345	12.863		1.00 27.29	В
	ATOM .	4867	NH1		318	19.383	11.963	71.849	1.00 28.67	В
	MOTA	4868	NH2		318	20.036	14.124	71.429	1.00 25.94	В
	MOTA	4869	C	ARG	318	22.434	9.679	67.344	1.00 8.51	В
	MOTA	4870	0	ARG	318	21.418	9.412	66.720	1.00 10.84	В
10	MOTA	4871	N	ILE	319	23.445	10.339	66.799	1.00 5.66	В
- •	ATOM	4872	CA	ILE	319	23.352	10.766	65.410	1.00 5.05	• В
										_
	MOTA	4873	CB	ILE	319	24.591	11.627	65.014	1.00 5.19	В
	MOTA	4874		ILE	319	24.531	11.976	63.544	1.00 6.51	В
	MOTA	4875	CG1	ILE	319	24.603	12.935	65.826	1.00 5.47	₿
15	MOTA	4876	CD1	ILE	319	25.833	13.774	65.632	1.00 2.71	В
	MOTA	4877	С	ILE	319	23.227	9.551	64.460	1.00 3.03	В
	MOTA	4878		ILE	319	22.361	9.511	63.590	1.00 1.95	B
	MOTA									
		4879	N	LEU	320	24.067	8.540	64.657	1.00 4.41	В
20	MOTA	4880	CA	LEU	320	24.056	7.376	63.767	1.00 5.60	В
20	MOTA	4881	CB	LEU	320	25.490	6.931	63.451	1.00 2.81	В
	MOTA	4882	CG	LEU	320	- 26.437	7.964	62.845	1.00 2.57	В
	MOTA	4883	CD1	LEU	320	27.873	7.442	62.786	1.00 2.20	В
	MOTA	4884		LEU	320	25.955	8.334	61.476	1.00 1.00	В
	ATOM	4885	c	LEU	320	23.313	6.122	64.235	1.00 7.52	B
25		4886								
23	MOTA		0	LEU	320	23.620	5.045	63.776	1.00 7.94	· В
	MOTA	4887	N	GLN	321	22.306	6.258	65.094	1.00 10.60	. В
	ATOM	4888	CA	GLN	321	21.629	5.057	65.604	1.00 16.44	В
	ATOM	4889	CB	GLN	321	20.679	5.362	66.775	1.00 18.94	В
	MOTA	4890	CG	GLN	321	19.433	6.153	66.458	1.00 22.43	В
30	ATOM	4891	CD	GLN	321	18.593	6.391	67.707	1.00 25.16	В
- •	ATOM	4892		GLN	321	18.121	5.453	68.338	1.00 26.09	В
				GLN						
	ATOM	4893	NE2		321	18.418	7.658	68.071	1.00 26.05	В
	ATOM	4894	C	GLN	321	20.882	4.186	64.617	1.00 16.64	В
25	ATOM	4895	0	GLN	321	20.700	2.992	64.870	1.00 16.23	В
35	ATOM	4896	N	ASP	322	20.439	4.759	63.505	1.00 17.01	В.
	MOTA	4897	CA	ASP	322	19.762	3.931	62.521	1.00 19.03	В
	MOTA	4898	CB	ASP	322	18.952	4.755	61.535	1.00 20.75	В
	ATOM	4899	CG	ASP	322	17.983	3.896	60.727	1.00 22.50	В
40	MOTA	4900	OD1		322	17.835	4.125	59.506	1.00 24.17	₿
40	ATOM	4901		ASP	322	17.352	2.997	61.327	1.00 21:00	В
	MOTA	4902	С	ASP	322	20.803	3.139	61.722	1.00 20.46	В
	ATOM	4903	0	ASP	322	20.467	2.335	60.861	1.00 23.04	В
	MOTA	4904	N	SER	323	22.076	3.385	62.006	1.00 20.16	В
	ATOM	4905	CA	SER	323	23.164	2.670	61.353	1.00 18.88	В
45			CB							
73	MOTA	4906		SER	323	24.299	3.643	61.077	1.00 17.96	В
	MOTA	4907	OG	SER	323	23.842	4.642	60.187	1.00 18.62	В
	MOTA	4908	С	SER	323	23.625	1.518	62.259	1.00 18.52	В
	ATOM	4909	0	SER	323	24.368	0.647	61.838	1.00 19.83	В
	MOTA	4910	N	LEU	324	23.168	1.512	63.507	1.00 16.09	В
50	ATOM	4911	CA	LEU	324	23.541	0.449	64.420	1.00 16:61	В
	ATOM	4912	CB	LEU	324	24.257	1.026	65.648	1.00 15.87	В
	MOTA	4913	CG	LEU	324	25.679	1.595	65.539	1.00 14.59	В
	MOTA	4914		LEU	324	26.545	0.643	64.722	1.00 13.37	В
c c	MOTA	4915		LEU	324	25.649	2.965	64.909	1.00 11.67	В
55	ATOM	4916	C	LEU	324	22.300	-0.343	64.834	1.00 17.48	В
	ATOM	4917	0	LEU	324	21.651	-0.025	65.814	1.00 16.83	В
	MOTA	4918	N	GLY	325	21.983	-1.387	64.071	1.00 17.97	В
	ATOM	4919	CA	GLY	325	20.818	-2.203	64.377	1.00 18.49	В
	MOTA	4920	Ċ.	GLY	325		-1.576	63.939		
60						19.498			1.00 19.29	В
UU	MOTA	4921	0	GLY	325	18.427	-1.950	64.423	1.00 19.24	В
	ATOM	4922	N	GLY	326	19.573	-0.630	63.007	1.00 19.01	В
	ATOM	4923	CA	GLY	326	18.382	0.052	62.539	1.00 18.79	В
	ATOM	4924	С	GLY	326	17.935	-0.373	61.165	1.00 19.04	В
	ATOM	4925	ō	GLY	326	17.931	-1.550	60.861	1.00 18.81	B
65	MOTA	4926	Ň	ARG	327	17.565	0.603	60.341	1.00 19.26	В
J.J										
	MOTA	4927	CA	ARG	327	17.106	0.336	58.991	1.00 20.71	В
	MOTA	4928	CB	ARG	327	15.731	0.970	58.761	1.00 22.28	В
	ATOM	4929	CG	ARG	327	14.591	0.225	59.443	1.00 25.87	В
~^	MOTA	4930	CD	ARG	327	13.233	0.703	58.976	1.00 28.38	В
70	MOTA	4931	NE	ARG	327	12.260	-0.388	58.957	1.00 33.27	В
	ATOM	4932	CZ	ARG	327	12.370	-1.477	58.193	1.00 36.86	В
	ATOM	4933	NH1		327	13.412	-1.639	57.382	1.00 38.23	В
	MOTA	4934	NH2		327	11.422		58.213		В
	VION	4224	14116	MO	361	11.462	-2.399	J4. ET3	1.00 38.97	ь

	MOTA	4935	С	ARG	327	18.072	0.784	57.899	1.00 20.64	В
	MOTA	4936	0	ARG	327	17.721	0.788	56.718	1.00 19.55	В
	MOTA	4937	N	THR	328	19.295	1.127	58.293	1.00 19.88	В
_	MOTA	4938	CA	THR	328	20.316	1.568	57.349	1.00 18.38	В
5	MOTA	4939	CB	THR	328	21.133	2.694	57.948	1.00 16.59	В
	ATOM	4940	OG1		328	20.260	3.780	58.254	1.00 15.01	В
	MOTA	4941	CG2		328	22.170	3.171	56.975	1.00 16.39	В
	MOTA	4942	С	THR	328	21.271	0.449	56.971	1.00 17.88	В
10	ATOM	4943	0	THR	328	21.640	-0.343	57.808	1.00 18.85	В
10	ATOM	4944	N	ARG	329	21.659	0.380	55.701	1.00 18.85	В
	MOTA	4945	·CA	ARG	329	22.605	-0.648	55.284	1.00 18.48	В
	MOTA	4946	CB	ARG	329	22.644	-0.784	53.756	1.00 21.31	В
	MOTA	4947	CG	ARG	329	23.540	-1.929	53.249	1.00 27.66	В
15	MOTA	4948	CD	ARG	329	23.818	-1.771	51.748	1.00 32.45	В
13	MOTA	4949	NE	ARG	329	24.651	-2.837	51.190	1.00 38.68	В
•	MOTA	4950	CZ	ARG ARG	329 329	25.871 26.417	-3.147 -2.476	51.626 52.641	1.00 43.03 1.00 45.11	B B
	ATOM ATOM	4951 4952		ARG	329	26.553	-4.122	51.032	1.00 45.11	В
	ATOM	4953	C	ARG	329	23.937	-0.161	55.840	1.00 14.99	В
20	ATOM	4954	ō	ARG	329	24.361	0.948	55.568	1.00 16.21	В
	ATOM	4955	N	THR	330	24.595	-0.987	56.632	1.00 12.23	В
	ATOM	4956	CA	THR	330	25.842	-0.559	57.235	1.00 11.36	₽.
	ATOM	4957	СВ	THR	330	25.720	-0.515	58.801	1.00 11.85	B
	ATOM	4958		THR	330	24.663	0.378	59.185	1.00 12.21	·B
25	MOTA	4959		THR	330	27.022	-0.038	59.432	1.00 10.17	В
	ATOM	4960	C	THR	330	27.031	-1.424	56.857	1.00 11.32	В
	ATOM	4961	0	THR	330	26.909	-2.639	56.699	1.00 11.14	В
	ATOM	4962	N	SER	331	28.176	-0.760	56.722	1.00 10.11	В
	MOTA	4963	CA	SER	331	29.432	-1.390	56.396	1.00 9.70	В
30	MOTA	4964	CB	SER	331	29.762	-1.121	54.938	1.00 10.15	В
	MOTA	4965	OG	SER	331	29.612	-2.305	54.201	1.00 16.41	В
	ATOM	4966	С	SER	331	30.551	-0.861	57.292	1.00 8.79	В
	MOTA	4967	0	SER	331	30.612	0.314	57.575	1.00 10.25	В
25	MOTA	4968	N	ILE	332	31.421	-1.744	57.761	1.00 7.54	В
35	ATOM '	4969	CA	ILE	332	32.537	-1.309	58.580	1.00 5.00	В
•	MOTA	4970	CB	ILE	332	32.484	-1.896	59.997	1.00 3.72	В
	MOTA	4971		ILE	332	33.791	-1.623	60.719	1.00 1.00	В
	ATOM	4972		ILE .			-1.308	60.755	1.00 1.20	В
40	MOTA	4973		ILE	332	31.044	-1.996	62.080	1.00 1.00	В
70	ATOM ATOM	4974 4975	0	ILE ILE	332 332	33.825 33.959	-1.761 -2.921	57.915 57.505	1.00 6.57 1.00 6.08	B B
	ATOM	4976	N	ILE	333	34.754	-0.824	57.779	1.00 6.74	В
	ATOM	4977	CA	ILE	333	36.052	-1.110	57.203	1.00 7.94	В
	ATOM	4978	CB	ILE	333	36.377	-0.134	56.043	1.00 7.86	В
45	ATOM	4979		ILE	333	37.745	-0.446	55.482	1.00 10.20	В
	ATOM	4980		ILE	333	35.335	-0.292	54.935	1.00 9.26	В
	ATOM	4981		ILE	333	35.562	0.532	53.743	1.00 9.53	В
	MOTA	4982	С	ILE	333	37.050	-0.961	58.362	1.00 9.22	В
	MOTA	4983	0	ILE	333	37.318	0.139	58.833	1.00 9.93	В
50	MOTA	4984	N	ALA	334	37.568	-2.087	58.842	1.00 9.27	В
	MOTA	4985	CA	ALA	334	38.510	-2.064	59.950	1.00 9.36	В
	MOTA	4986	CB	ALA		. 38.318	-3.281	60.815	1.00 8.99	В
	MOTA	4987	С	ALA	334	39.914	-2.033	59.366	1.00 9.97	В
55	MOTA	4988	0	ALA	334	40.289	-2.887	58.558	1.00 9.97	В
55	MOTA	4989	N	THR	335	40.689	-1.039	59.780	1.00 10.59	В
	MOTA	4990	CA	THR	335	42.041	-0.877	59.267	1.00 11.33	В
	ATOM	4991	CB	THR	335	42.300	0.587	58.833	1.00 11.54	В
	MOTA	4992		THR	335	42.165	1.471	59.959	1.00 11.31	₿.
60	ATOM	4993		THR	335	41.316	0.973	57.707	1.00 10.89	В
UU	MOTA	4994	C	THR	335	43.059	-1.311	60.297	1.00 11.80	В
	MOTA	4995	0	THR	335	42.898	-1.044	61.479	1.00 11.91	В
	MOTA	4996	N	ILE	336	44.108	-1.981	59.825	1.00 10.99	В
	MOTA	4997	CA	ILE	336	45.150	-2.494	.60.691	1.00 9.23	В
65	MOTA	4998	CB	ILE	336 336	44.988 43.726	-4.002	60.867	1.00 6.21	В
05	MOTA MOTA	4999 5000		ILE	336 336	44.949	-4.275	61.631	1.00 2.30 1.00 4.99	В
	ATOM	5000		ILE	336 336	44.977	-4.688 -6.187	59.501 59.570	1.00 4.99 1.00 4.80	B B
	ATOM	5001	CDI	ILE	336	46.549	-0.187	60.175	1.00 4.80	B B
	MOTA	5002	Ö	ILE	336	46.722	-1.683	59.054	1.00 12.29	B
70	MOTA	5004	N	SER	337	47.536	-2.533	61.011	1.00 15.10	В
-	MOTA	5005	CA	SER	337	48.958	-2.344	60.716	1.00 17.38	В
	MOTA	5006	CB	SER	337	49.673	-1.619	61.848	1.00 16.32	B
	MOTA	5007	OG	SER	337	51.071	-1.842	61.757	1.00 15.90	B

	MOTA	5008	•	CED	337	49.690	-3.686	60.569	1 00 10 52	
			Ç	SER					1.00 18.53	В
	ATOM	5009	0	SER	337	49.393	-4.652	61.292	1.00 19.54	В
	MOTA MOTA	5010	N	PRO	338	50.643	-3.770	59.618	1.00 17.27	В
5		5011	CD	PRO	338	50.949.	-2.790	58.555	1.00 15.95	В
J	MOTA	5012	CA	PRO	338	51.398	-5.005	59.403	1.00 15.90	В
	MOTA	5013	CB	PRO	338	51.851	-4.868	57.953	1.00 14.63	В
	ATOM	5014	CG	PRO	338	52.158	-3.420	57.858	1.00 15.30	В
	ATOM	5015	C	PRO	338	52.574	-5.124	60.360	1.00 15.45	В
10	MOTA	5016	0	PRO	338	53.206		60.420	1.00 15.18	В
10	MOTA	5017	N	ALA	339	52.844	-4.053	61.103	1.00 16.79	В
	MOTA	5018	CA	ALA	339	53.986	-3.999	62.025	1.00 19.03	· В
	MOTA	5019	CB	ALA	339	54.296	-2.536	62.409	1.00 17.80	В
	ATOM	5020	С	ALA	339	53.813	-4.824	63.277	1.00 19.74	В
1.5	ATOM	5021	0	ALA	339	52.727	-4.883	63.824	1.00 21.39	В
15	MOTA	5022	N	SER	340	54.896	-5.452	63.734	1.00 20.20	В
	ATOM	5023	CA	SER	340	54.825	-6.278	64.940	1.00 20.54	В
	ATOM	5024	CB	SER	340	56.045	-7.193	65.075	1.00 21.46	В
	MOTA	5025	OG	SER	340	57.233	-6.430	65.182	1.00 24.93	В
00	ATOM	5026	С	SER	340	54:727	-5.453	66.208	1.00 19.22	В
20	MOTA	5027	0	SER	340	54.293	-5.941	67.224	1.00 17.09	В
	MOTA	5028	N	LEU	341	. 55.131	-4.191	66.143	1.00 20.29	В
	MOTA	5029	CA	LEU	341	55.048	-3.345	67.328	1.00 21.64	В
	ATOM	5030	CB	LEU	341	56.040	-2.184	67.248	1.00 23.99	В
	MOTA	5031	CG	LEU	341	55.610	-0.896	66.546	1.00 27.23	В
25	ATOM	5032	CD1	LEU	341	55.641	0.269	67.554	1.00 26.67	В
	ATOM	5033	CD2	LEU	341	56.542	-0.630	65.357	1.00 28.22	. В
	ATOM	5034	С	LEU	341	53.629	-2.807	67.502	1.00 21.40	В
	MOTA	5035	0	LEU	341	53.350	-2.053	68.424	1.00 21.64	В
	MOTA	5036	N	ASN	342	52.736	-3.227	66.613	1.00 21.16	В
30	MOTA	5037	CA	ASN	342	51.335	-2.815	66.664	1.00 21.98	В
	MOTA	5038	CB	ASN	342	50.943	-2.165	65.352	1.00 20.54	В
	ATOM	5039	CG	ASN	342	51.586	-0.826	65.172	1.00 21.64	В
	MOTA	5040	OD1	ASN	342	51.897	-0.423	64.046	1.00 19.82	В
	ATOM	5041		ASN	342	51.785	-0.107	66.285	1.00 20.76	В
35	ATOM	5042	С	ASN	342	50.415	-4.011	66.892	1.00 22.33	В -
	ATOM	5043	ŏ	ASN	342	49.201	-3.909	66.761	1.00 22.21	В
	ATOM	5044	N	LEU	343	51.023	-5.135	67.254	1.00 23.56	В
	ATOM	5045	CA	LEU	343	50.334	-6.406	67.488	1.00 24.35	В
	ATOM	5046	CB	LEU	343	51.360	-7.435	67.992	1.00 25.91	В
40	ATOM	5047	CG	LEU	343	50.986	-8.890	68.316	1.00 28.30	В
. •	ATOM	5048		LEU	343	50.524	-8.995	69.761	1.00 29.51	В
	ATOM	5049		LEU	343	49.930	~9.392	67.334	1.00 28.29	В
	ATOM	5050	Ç	LEU	343	49.119	-6.347	68.412	1.00 22.80	В
	ATOM	5051	ŏ	LEU	343	48.024	-6.756	68.045	1.00 21.40	В
45	ATOM	5052	N	GLU	344	49.305	-5.831	69.614	1.00 23.08	В
	ATOM	5053	CA	GLU	344	48.189	-5.745	70.545	1.00 22.34	В
	ATOM	5054	СВ	GLU	344	48.628	-5.122	71.861	1.00 24.68	В
	ATOM	5055	CG	GLU	344	47.491	-4.875	72.821	1.00 30.10	В
	ATOM	5056	CD	GLU	344	47.965	-4.715	74.263	1.00 34.59	.B
50	ATOM	5057	OE1		344	48.866	-3.886	74.538	1.00 36.85	В
-	ATOM	5058		GLU	344	47.422	-5.428	75.134	1.00 36.33	В
	ATOM	5059	č	GLU	344	47.002	-4.960	70.002	1.00 19.86	В
	ATOM	-5060	õ	GLU	344	45.894	-5.425	70.097	1.00 20.25	В
	ATOM	5061	N	GLU	345	47.241	-3.770	69.452	1.00 17.13	В
55	ATOM	5062	CA	GLU	345	46.141	-2.974	68.907	1.00 16.35	В
	ATOM	5063	CB	GLU	345	46.585	-1.527	68.589	1.00 15.68	В
	ATOM	5064	CG	GLU	345	46.803	-0.645	69.824	1.00 13.57	В
	ATOM	5065	CD	GLU	345	45.528	-0.391	70.618	1.00 13.00	В
	MOTA	5066		GLU	345	45.623	0.062	71.768		В
60	MOTA	5067		GLU	345	44.419	-0.628	70.111	1.00 14.32 1.00 13.44	
00	ATOM	5068	C	GLU	345	45.528				В
							-3.626	67.659	1.00 14.78	В
	MOTA MOTA	5069 5070	N N	GLU TUD	345 346	44.326	-3.544	67.442	1.00 14.79	В
	ATOM			THR	346 346	46.350	-4.284	66.846	1.00 14.54	В
65		5071	CA	THR	346	45.863	-4.959	65.641	1.00 14.71 1.00 15.75	. B
5 5	MOTA	5072	CB	THR	346	47.046	-5.572	64.839		В
	MOTA	5073		THR	346	47.870	-4.523	64.301	1.00 19.38	В
	MOTA	5074		THR	346	46.520	-6.467	63.721	1.00 15.93	В
	ATOM .	5075	C	THR	346	44.888	-6.075	66.057	1.00 14.75	В
70	MOTA	5076	0	THR	346	43.863	-6.320	65.403	1.00 12.97	В
70	ATOM	5077	N	LEU	347	45.210	-6.741	67.165	1.00 15.11	В
	ATOM	5078	CA	LEU	347	44.371	-7.819	67.693	1.00 14.94	В
	ATOM	5079	CB	LEU	347	45.080	-8.601	68.797	1.00 13.17	В
	MOTA	5080	CG	LEU	347	46.253	-9.465	68.342	1.00 12.75	В

ATOM 5081 CD1 LEU 347 45.781 -10.156 69.559 1.00 9.82 B ATOM 5082 CD2 LEU 347 45.781 -10.256 67.281 1.00 10.19 B ATOM 5083 C LEU 347 42.033 -7.935 68.277 1.00 14.55 B ATOM 5083 C LEU 347 42.033 -7.935 68.277 1.00 14.55 B ATOM 5086 C SER 348 42.236 -4.288 70.244 1.00 11.65 B ATOM 5087 CS SER 348 42.236 -4.288 70.244 1.00 11.62 B ATOM 5089 CS SER 348 42.236 -4.288 70.244 1.00 11.62 B ATOM 5089 CS SER 348 40.974 -5.180 68.033 1.00 12.87 B ATOM 5099 C SER 348 39.809 -5.505 68.355 1.00 12.88 B ATOM 5091 N THR 349 41.595 -3.400 65.051 1.00 14.07 B ATOM 5092 CA THR 349 41.515 -3.400 65.081 1.00 14.87 B ATOM 5095 CT THR 349 41.515 -3.200 66.535 1.00 17.94 B ATOM 5095 CT THR 349 40.736 -5.323 66.81 1.00 14.87 B ATOM 5095 CT THR 349 40.736 -5.323 66.542 1.00 15.46 B ATOM 5095 C THR 349 39.922 -5.316 65.922 1.00 15.46 B ATOM 5099 CA LEU 350 40.777 -6.339 65.157 1.00 15.46 B ATOM 5099 C LEU 350 40.727 -6.339 65.157 1.00 15.46 B ATOM 5099 C LEU 350 40.727 -7.339 65.157 1.00 15.46 B ATOM 5099 C LEU 350 40.727 -7.339 65.157 1.00 15.46 B ATOM 5099 C LEU 350 40.727 -7.339 65.157 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.508 1.00 14.48 B ATOM 5090 C C THR 349 33.942 -5.316 64.508 1.00 14.48 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5090 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5000 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5000 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5000 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5000 C C THR 349 33.942 -5.316 64.958 1.00 15.46 B ATOM 5100 C C LEU 350 41.956 -8.950 64.950 1.00 12.90 B ATOM 5100 C C LEU 350 41.956 -8.950 64.950 1.00 12.90 B ATOM 5100 C C LEU 350 41.956 8.950 64.950 1.00 11.90 B ATO											
508 ATOM 5088 O. LEU 347 42.039 -7.935 68.277 1.00 14.55 B ATOM 5086 N SER 348 41.917 -5.314 69.425 1.00 14.94 B ATOM 5086 CS SER 348 42.236 -4.288 70.204 1.00 11.28 B ATOM 5088 O. SER 348 42.236 -4.288 70.204 1.00 11.28 B ATOM 5088 O. SER 348 42.236 -4.288 70.204 1.00 11.62 B ATOM 5088 O. SER 348 42.841 -4.656 71.416 1.00 11.62 B ATOM 5089 O. SER 348 42.841 -4.656 71.416 1.00 11.62 B ATOM 5089 O. SER 348 42.841 -4.656 71.416 1.00 11.62 B ATOM 5090 O. SER 348 39.809 -5.505 681.355 1.00 12.88 B ATOM 5091 N THR 349 41.515 -5.506 68.303 1.00 12.87 B ATOM 5092 CA THR 349 40.672 -4.121 661.51 1.00 14.07 B ATOM 5092 CA THR 349 41.515 -3.400 65.085 1.00 12.34 B ATOM 5092 CA THR 349 41.515 -3.400 65.085 1.00 14.07 B ATOM 5093 CO THR 349 41.515 -3.400 65.085 1.00 14.07 B ATOM 5093 CO THR 349 41.887 -3.93 65.255 1.00 17.94 B ATOM 5095 CO THR 349 99.992 -3.218 67.282 1.00 17.94 B ATOM 5095 CO THR 349 99.992 -3.23 67.282 1.00 17.94 B ATOM 5095 CO THR 349 99.992 -3.23 67.282 1.00 11.62 B ATOM 5099 CA LEU 350 40.226 -7.518 64.266 1.00 14.08 B ATOM 5099 CA LEU 350 40.226 -7.518 64.266 1.00 14.08 B ATOM 5090 CB LEU 350 40.226 -7.518 64.268 1.00 15.00 B ATOM 5100 CB LEU 350 40.226 -7.518 64.268 1.00 15.08 B ATOM 5101 CC LEU 350 41.963 8.99 64.206 1.00 14.08 B ATOM 5101 CC LEU 350 49.364 9.99 64.206 1.00 14.08 B ATOM 5101 CC LEU 350 49.364 9.99 64.206 1.00 14.08 B ATOM 5101 CC LEU 350 49.364 9.99 64.206 1.00 14.08 B ATOM 5101 CC LEU 350 49.364 9.99 64.206 1.00 14.08 B ATOM 5101 CC LEU 350 49.364 9.99 64.206 1.00 19.95 B ATOM 5101 CC LEU 350 40.226 -9.172 65.367 1.00 15.08 B ATOM 5101 CC LEU 350 40.226 -9.172 65.367 1.00 15.08 B ATOM 5101 CC LEU 350 40.226 -9.172 65.367 1.00 15.08 B ATOM 5101 CC LEU 350 40.226 -9.172 65.367 1.00 15.08 B ATOM 5101 CC LEU 350 40.266 -9.172 65.367 1.00 15.88 B ATOM 5101 CC LEU 350 40.266 -9.172 65.367 1.00 15.98 B ATOM 5101 CC LEU 350 40.266 -9.172 65.367 1.00 19.91 B ATOM 5101 CC LEU 350 40.266 -9.172 65.367 1.00 19.91 B ATOM 5101 CC LEU 350 40.266 40.90 40.266 40.90 10.00 19.91 B ATOM 5101 CC LEU		MOTA	5081			347			69.559	1.00 9.82	В
SATOM 5084 O LEU 347		•									В
50 ATOM 5085 N SER 348 41.917 -6.107 68.872 1.00 14.94 B ATOM 5086 CS SER 348 42.236 -4.288 70.204 1.00 11.62 B ATOM 5080 CS SER 348 42.236 -4.288 70.204 1.00 11.62 B ATOM 5080 CS SER 348 42.814 -4.656 71.416 1.00 11.62 B ATOM 5080 CS SER 348 39.809 -5.505 68.355 1.00 12.88 B ATOM 5091 N THR 349 40.974 -5.180 68.303 1.00 12.87 B ATOM 5092 CD THR 349 40.672 -4.121 66.151 1.00 12.34 B ATOM 5092 CD THR 349 40.672 -4.121 66.151 1.00 12.34 B ATOM 5093 CB THR 349 40.672 -4.121 66.151 1.00 14.07 B ATOM 5093 CB THR 349 40.572 -4.121 66.151 1.00 14.07 B ATOM 5095 CG2 THR 349 40.738 -2.398 66.1535 1.00 17.94 B ATOM 5095 CG2 THR 349 40.738 -2.398 66.1535 1.00 17.94 B ATOM 5095 CG2 THR 349 39.992 -5.338 66.1281 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5095 CG2 THR 349 39.992 -5.338 66.282 1.00 15.16 B B ATOM 5005 CG2 CD1 LEU 350 40.226 -7.518 46.508 1.00 15.16 B B ATOM 5101 CG LEU 350 40.226 -7.518 46.508 1.00 15.08 B ATOM 5103 CC2 LEU 350 40.226 -7.518 66.282 1.00 15.08 B B ATOM 5103 CC2 LEU 350 40.226 -7.518 66.290 1.00 14.08 B ATOM 5103 CC2 LEU 350 40.226 -7.518 66.206 1.00 14.08 B ATOM 5103 CC2 LEU 350 40.226 -7.518 66.206 1.00 14.08 B ATOM 5103 CC2 LEU 350 40.226 CB2 50.00 10.00 12.88 B ATOM 5103 CC2 LEU 350 40.226 CB2 50.00 10.00 12.88 B ATOM 5103 CC2 LEU 350 40.226 CB2 50.00 10.00 12.89 B ATOM 5103 CC2 LEU 350 40.226 CB2 50.00 10.00 12.89 B ATOM 5107 CC2 CD1 LEU 350 ADOM 5107 CC2 CD1 LEU 350 ADOM 5107 CC2 CD1 L											В
ATOM 5086 CA SER 348 42.23 6-5.54 69.425 1.00 12.86 B ATOM 5087 CB SER 348 42.841 -4.656 71.416 1.00 11.62 B B ATOM 5089 C SER 348 40.974 -5.180 68.303 1.00 12.87 B ATOM 5089 C SER 348 40.974 -5.180 68.303 1.00 12.87 B ATOM 5091 N THR 349 41.494 -4.518 67.281 1.00 12.88 B ATOM 5092 CA THR 349 40.672 -4.121 66.151 1.00 14.07 B ATOM 5093 CB THR 349 41.595 -3.400 65.081 1.00 14.87 B ATOM 5093 CB THR 349 41.595 -3.400 65.081 1.00 14.87 B ATOM 5095 CC THR 349 40.573 -3.283 65.083 1.00 15.48 B ATOM 5095 CC THR 349 40.573 -3.232 65.083 1.00 15.48 B ATOM 5095 CC THR 349 40.573 -3.232 65.282 1.00 15.48 B ATOM 5095 CC THR 349 40.738 -3.238 63.883 1.00 15.48 B ATOM 5095 CC THR 349 38.770 -5.325 65.282 1.00 15.48 B ATOM 5097 CD THR 349 38.770 -5.325 65.282 1.00 15.48 B ATOM 5099 CD THR 349 38.770 -5.325 65.282 1.00 15.82 B ATOM 5099 CD THR 349 38.770 -5.325 65.282 1.00 15.82 B ATOM 5099 CD LEU 350 40.226 -7.518 64.508 1.00 15.08 B ATOM 5099 CD LEU 350 40.226 -7.518 64.508 1.00 15.08 B ATOM 5099 CD LEU 350 40.226 -7.518 64.508 1.00 15.08 B ATOM 5090 CD LEU 350 40.226 -7.518 64.508 1.00 10.95 B ATOM 5100 CD LEU 350 41.352 -8.856 64.206 1.00 10.95 B ATOM 5100 CD LEU 350 41.352 -8.856 64.206 1.00 10.95 B ATOM 5100 CD LEU 350 41.352 -8.856 64.206 1.00 10.95 B ATOM 5100 CD LEU 350 40.226 -7.518 66.508 1.00 10.95 B ATOM 5106 N GUJ 351 39.443 -8.254 66.658 1.00 10.95 B ATOM 5106 N GUJ 351 39.443 -8.254 66.658 1.00 10.95 B ATOM 5106 N GUJ 351 39.443 -8.254 66.658 1.00 10.95 B ATOM 5106 N GUJ 351 39.443 -8.254 66.658 1.00 10.82 B ATOM 5102 CD GUJ 351 39.444 -8.846 69.003 1.00 21.84 B ATOM 5110 CD GUJ 351 39.441 -8.846 69.003 1.00 21.84 B ATOM 5110 CD GUJ 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 CD GUJ 351 39.441 -8.846 69.003 1.00 19.87 B ATOM 5112 CD GUJ 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 CD GUJ 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 CD GUJ 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 CD GUJ 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 CD GUJ 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 C	_	MOTA	5084	0	LEU	347	42.039	-7.935	68.196	1.00 16.59	В
ATOM 5088 OS SER 348 42.236 -4.288 70.204 1.00 11.62 B ATOM 5088 OS SER 348 42.836 -4.286 11.465 61.71.446 1.00 18.29 B ATOM 5090 C SER 348 39.809 -5.505 68.355 1.00 12.88 B ATOM 5091 N THR 349 40.974 -5.180 68.303 1.00 12.87 B ATOM 5092 CA THR 349 40.974 -5.180 68.303 1.00 12.87 B ATOM 5092 CA THR 349 40.974 -5.180 67.281 1.00 12.34 B ATOM 5093 CB THR 349 40.972 -4.121 66.151 1.00 12.34 B ATOM 5094 CG THR 349 40.572 -4.121 66.151 1.00 14.07 B ATOM 5095 CG2 THR 349 40.738 -3.238 63.828 1.00 14.87 B ATOM 5095 CG2 THR 349 40.738 -3.238 63.828 1.00 15.48 B ATOM 5096 CG2 THR 349 39.992 -5.321 65.535 1.00 16.16 B ATOM 5096 CG2 THR 349 39.992 -5.321 65.493 1.00 16.16 B ATOM 5096 CG2 THR 349 39.992 -5.321 65.493 1.00 15.48 B ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5099 CA LEU 350 40.727 -6.339 65.157 1.00 15.00 B ATOM 5099 CA LEU 350 40.727 -6.339 64.206 1.00 15.08 B ATOM 5100 CB LEU 350 41.953 -8.496 64.206 1.00 14.08 B ATOM 5100 CB LEU 350 41.953 -8.496 64.206 1.00 14.08 B ATOM 5102 CDL LEU 350 41.953 -8.496 64.206 1.00 10.81 B ATOM 5102 CDL LEU 350 41.953 -8.496 64.206 1.00 10.80 B ATOM 5102 CDL LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5102 CDL LEU 350 42.004 -7.143 62.947 1.00 10.95 B ATOM 5104 C LEU 350 391.62 -8.172 65.367 1.00 10.81 B ATOM 5104 C LEU 350 391.62 -8.172 65.367 1.00 10.81 B ATOM 5106 C C CLU 351 391.44 -8.466 66.658 1.00 10.81 B ATOM 5106 C C CLU 351 391.44 -8.466 66.658 1.00 10.82 B ATOM 5106 C C CLU 351 391.44 -8.466 66.658 1.00 10.82 B ATOM 5106 C C CLU 351 391.44 -8.466 66.658 1.00 10.82 B ATOM 5106 C C CLU 351 391.44 -8.466 66.658 1.00 10.82 B ATOM 5110 C C CLU 351 391.44 -8.466 66.658 1.00 11.22 B ATOM 5110 C C CLU 351 391.44 -8.466 66.658 1.00 11.22 B ATOM 5111 C C C CLU 351 391.44 -8.466 66.658 1.00 11.22 B ATOM 5110 C C C CLU 351 391.44 -8.466 66.658 1.00 11.82 B ATOM 5110 C C C C C C C C C C C C C C C C C C	2	MOTA	5085	N	SER	348	43.127	-6.107	68.872	1.00 14.94	В
ATOM 5088 OS SER 348 40,974 -5.180 68.303 1.00 12.87 B ATOM 5099 OS SER 348 40,974 -5.180 68.303 1.00 12.87 B ATOM 5091 N THR 349 41.594 -4.518 67.281 1.00 12.88 B ATOM 5092 CA THR 349 41.594 -4.518 67.281 1.00 12.34 B ATOM 5093 CB THR 349 41.595 -3.400 65.081 1.00 14.87 B ATOM 5095 CG THR 349 41.595 -3.400 65.081 1.00 14.87 B ATOM 5095 CG THR 349 41.587 -3.240 65.081 1.00 15.48 B ATOM 5095 CG THR 349 40.738 -3.238 63.828 1.00 15.48 B ATOM 5095 CG THR 349 40.738 -3.238 63.828 1.00 15.48 B ATOM 5095 CG THR 349 40.738 -3.238 63.828 1.00 15.48 B ATOM 5097 CT THR 349 38.770 -5.325 65.282 1.00 15.48 B ATOM 5098 N LEU 350 40.226 -7.518 65.493 1.00 15.08 B ATOM 5099 CA LEU 350 40.226 -7.518 64.598 1.00 15.08 B ATOM 5099 CA LEU 350 40.226 -7.518 64.598 1.00 15.08 B ATOM 5099 CA LEU 350 41.963 -8.503 62.947 1.00 10.95 B ATOM 5102 CD LEU 350 41.963 -8.503 62.947 1.00 10.95 B ATOM 5102 CD LEU 350 39.147 -9.03 62.947 1.00 10.95 B ATOM 5106 C LEU 350 39.147 -9.03 62.947 1.00 10.95 B ATOM 5106 C LEU 350 39.132 -8.595 64.876 1.00 17.88 B ATOM 5106 C LEU 350 39.132 -8.595 64.876 1.00 17.88 B ATOM 5106 C LEU 350 39.132 -8.595 64.876 1.00 19.87 B ATOM 5106 C LEU 351 39.441 -8.846 69.003 1.00 10.82 B ATOM 5102 C LEU 351 39.441 -8.846 69.003 1.00 19.87 B ATOM 5102 C LEU 351 39.481 -11.771 69.051 1.00 19.87 B ATOM 5112 C LEU 351 39.481 -11.771 69.051 1.00 19.87 B ATOM 5112 C LEU 351 39.481 -11.771 69.051 1.00 19.87 B ATOM 5112 C LEU 351 39.481 -11.771 69.		ATOM	5086	CA	SER	348	41.917	-5.534	69.425	1.00 12.88	В
10 ATOM 5099 C SER 348 39.809 -5.505 68.355 1.00 12.88 B ATOM 5091 N THR 349 41.494 -4.518 67.281 1.00 12.34 B ATOM 5091 N THR 349 40.572 -4.121 66.151 1.00 12.34 B ATOM 5092 CA THR 349 40.572 -4.121 66.151 1.00 12.34 B ATOM 5093 CB THR 349 40.572 -4.121 66.151 1.00 14.07 B ATOM 5094 CG THR 349 41.515 -3.400 65.081 1.00 14.87 B ATOM 5095 CG2 THR 349 40.738 -3.238 63.828 1.00 15.94 B ATOM 5095 CG2 THR 349 40.738 -3.238 63.828 1.00 15.48 B ATOM 5095 CG2 THR 349 39.9992 -5.321 65.493 1.00 16.16 B ATOM 5096 N THR 349 39.9992 -5.321 65.493 1.00 15.48 B ATOM 5096 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5098 N LEU 350 40.727 -6.339 64.206 1.00 15.08 B ATOM 5000 E LEU 350 40.266 -7.518 64.206 1.00 14.08 B ATOM 5100 CB LEU 350 41.953 -8.496 64.206 1.00 14.08 B ATOM 5102 CD LEU 350 41.953 -8.496 64.206 1.00 14.08 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.81 B ATOM 5102 CD LEU 350 391.62 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 66.658 1.00 17.28 B ATOM 5106 CB CGU 351 391.462 -9.496 66.588 1.00 19.22 B ATOM 5106 CB CGU 351 391.462 -9.496 66.588 1.00 19.22 B ATOM 5106 CB CGU 351 391.462 -9.496 66.588 1.00 19.25 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19		MOTA	5087	CB	SER	348	42.236	-4.288	70.204	1.00 11.62	В
10 ATOM 5099 C SER 348 39.809 -5.505 68.355 1.00 12.88 B ATOM 5091 N THR 349 41.494 -4.518 67.281 1.00 12.34 B ATOM 5091 N THR 349 40.572 -4.121 66.151 1.00 12.34 B ATOM 5092 CA THR 349 40.572 -4.121 66.151 1.00 12.34 B ATOM 5093 CB THR 349 40.572 -4.121 66.151 1.00 14.07 B ATOM 5094 CG THR 349 41.515 -3.400 65.081 1.00 14.87 B ATOM 5095 CG2 THR 349 40.738 -3.238 63.828 1.00 15.94 B ATOM 5095 CG2 THR 349 40.738 -3.238 63.828 1.00 15.48 B ATOM 5095 CG2 THR 349 39.9992 -5.321 65.493 1.00 16.16 B ATOM 5096 N THR 349 39.9992 -5.321 65.493 1.00 15.48 B ATOM 5096 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5098 N LEU 350 40.727 -6.339 64.206 1.00 15.08 B ATOM 5000 E LEU 350 40.266 -7.518 64.206 1.00 14.08 B ATOM 5100 CB LEU 350 41.953 -8.496 64.206 1.00 14.08 B ATOM 5102 CD LEU 350 41.953 -8.496 64.206 1.00 14.08 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.81 B ATOM 5102 CD LEU 350 391.62 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 65.367 1.00 11.99 B ATOM 5106 CB CGU 351 391.462 -8.172 66.658 1.00 17.28 B ATOM 5106 CB CGU 351 391.462 -9.496 66.588 1.00 19.22 B ATOM 5106 CB CGU 351 391.462 -9.496 66.588 1.00 19.22 B ATOM 5106 CB CGU 351 391.462 -9.496 66.588 1.00 19.25 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19.57 B ATOM 5110 CD CGU 351 391.462 -9.496 69.659 1.00 19		MOTA	5088	OG	SER	348	42.841	-4.656	71.416		
10 ATOM 5090 O SER 348 39,809 -5.505 68.355 1.00 12.84 B ATOM 5091 N THR 349 41.694 -4.518 67.281 1.10 12.34 B ATOM 5093 CA THR 349 41.697 -2.4121 66.151 1.00 14.07 B ATOM 5093 CB THR 349 41.887 -2.906 65.081 1.10 14.07 B ATOM 5095 CG THR 349 41.887 -2.096 65.081 1.10 14.87 B ATOM 5095 CG THR 349 41.887 -2.096 65.081 1.10 10 15.48 B ATOM 5095 CG THR 349 40.738 -3.238 63.828 1.10 15.48 B ATOM 5095 CG THR 349 40.738 -3.238 65.282 1.10 15.48 B ATOM 5097 CM THR 349 38.770 -5.325 65.282 1.10 15.48 B ATOM 5099 CA LEU 350 40.777 -6.339 65.187 1.00 15.08 B ATOM 5099 CA LEU 350 40.777 -6.339 65.187 1.00 15.08 B ATOM 5101 CG LEU 350 41.352 -8.496 64.206 1.00 15.08 B ATOM 5101 CG LEU 350 41.352 -8.496 64.206 1.00 10.95 ATOM 5103 CD LEU 350 41.352 -8.496 64.206 1.00 10.95 ATOM 5103 CD LEU 350 43.347 -9.038 62.241 1.00 10.81 B ATOM 5103 CD LEU 350 43.347 -9.038 62.241 1.00 10.81 B ATOM 5103 CD LEU 350 43.347 -9.038 62.247 1.00 11.99 B ATOM 5105 CD LEU 350 38.132 -8.595 64.876 1.00 17.28 B ATOM 5105 CD LEU 350 38.132 -8.595 64.876 1.00 17.28 B ATOM 5105 CD LEU 350 38.132 -8.595 64.876 1.00 17.28 B ATOM 5107 CD LEU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5107 CD LEU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5107 CD LEU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5107 CD CLU 351 38.420 -11.196 69.403 1.00 21.84 B ATOM 5101 CD CLU 351 38.440 -9.791 69.955 1.00 26.42 B ATOM 5110 CD CLU 351 38.440 -9.791 69.955 1.00 20.64 2 B ATOM 5111 CD CLU 351 38.440 -9.791 69.955 1.00 20.64 2 B ATOM 5111 CD CLU 351 39.441 -8.842 67.609 1.00 10.95 B B ATOM 5111 CD CLU 351 39.441 -8.842 69.093 1.00 32.89 B ATOM 5111 CD CLU 351 39.441 -8.842 69.093 1.00 32.89 B ATOM 5112 CD CLU 351 39.441 -8.842 69.093 1.00 32.89 B ATOM 5113 CD CLU 351 39.441 -8.842 69.093 1.00 32.89 B ATOM 5113 CD CLU 371 352 36.816 -0.703 67.641 1.00 19.57 B ATOM 5112 CD CLU 371 352 37.566 -0.703 67.641 1.00 19.57 B ATOM 5112 CD CLU 371 352 37.566 -0.703 67.641 1.00 19.53 B ATOM 5112 CD CLU 371 352 37.566 -0.703 67.641 1.00 10.12 B ATOM 5112 CD CLU 371 352 37.566 -0.703 67.											
ATOM 5091 N THR 349 40.672 -4.121 66.151 1.00 12.34 B ATOM 5092 CB THR 349 40.672 -4.121 66.151 1.00 14.07 B ATOM 5094 CG THR 349 41.515 -3.400 65.081 1.00 14.87 B ATOM 5095 CG2 THR 349 40.738 -3.238 63.288 1.00 15.48 B ATOM 5095 CC2 THR 349 40.738 -3.238 63.288 1.00 15.48 B ATOM 5095 CC THR 349 39.992 -5.321 65.493 1.00 16.16 B ATOM 5096 C THR 349 39.992 -5.325 65.282 1.00 15.48 B ATOM 5097 O THR 349 39.770 -5.325 65.282 1.00 15.82 B ATOM 5099 CA LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5100 CG LEU 350 40.226 -7.518 64.508 1.00 15.08 B ATOM 5100 CG LEU 350 41.953 -8.503 62.812 1.00 10.95 B ATOM 5102 CD LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.81 B ATOM 5102 CD LEU 350 43.347 -9.038 62.947 1.00 11.99 B ATOM 5103 CD2 LEU 350 39.162 8.172 65.367 1.00 15.08 B ATOM 5100 CD LEU 350 39.162 8.172 65.367 1.00 16.08 B ATOM 5100 CD LEU 350 39.162 8.172 65.367 1.00 16.98 B ATOM 5106 CD LEU 350 39.162 8.172 65.367 1.00 16.98 B ATOM 5106 CD LEU 350 39.162 8.172 65.367 1.00 16.48 B ATOM 5106 CD GLU 351 39.443 8.254 66.558 1.00 18.22 B ATOM 5106 CD GLU 351 39.443 8.254 66.558 1.00 18.22 B ATOM 5106 CD GLU 351 39.444 8.846 66.508 1.00 19.87 B ATOM 5100 CD GLU 351 38.514 -8.842 67.509 1.00 19.87 B ATOM 5100 CD GLU 351 39.441 -8.846 66.500 1.00 19.87 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 39.481 1.771 69.051 1.00 29.53 B ATOM 5110 CD GLU 351 352 30.00 3	10										
ATOM 5092 CA THR 349 40.672 -4.121 66.151 1.00 14.07 B ATOM 5094 CGI THR 349 41.887 -2.096 65.081 1.00 17.94 B ATOM 5095 CC THR 349 40.738 -3.238 65.535 1.00 17.94 B ATOM 5095 CC THR 349 39.992 -5.321 65.493 1.00 16.16 B ATOM 5097 O THR 349 39.992 -5.321 65.493 1.00 16.16 B ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5099 CO LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5099 CO LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5100 CB LEU 350 40.266 -7.518 64.508 1.00 15.08 B ATOM 5101 CC LEU 350 41.352 -8.496 64.206 1.00 14.08 B ATOM 5102 CD1 LEU 350 42.046 -7.143 62.214 1.00 10.81 B ATOM 5103 CC LEU 350 39.162 -8.172 65.367 1.00 15.95 B ATOM 5104 C LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5105 O LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5105 CD LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5105 CD LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5105 CD LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5105 CD LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5107 CA GLU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5108 CB GLU 351 39.444 -8.846 69.003 1.00 21.84 B ATOM 5109 CC GLU 351 39.449 -9.791 69.965 1.00 21.84 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 21.84 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 25.42 B ATOM 5111 CEI GLU 351 39.481 11.771 69.051 1.00 29.53 B ATOM 5112 CEZ GLU 351 37.289 11.724 69.309 1.00 32.89 B ATOM 5117 CB TTR 352 35.768 -6.766 67.04 1.00 19.57 B ATOM 5116 CA TTR 352 35.06 6.676 67.04 1.00 11.73 B ATOM 5117 CB TTR 352 35.06 6.676 67.04 1.00 11.73 B ATOM 5118 CG TTR 352 35.06 6.676 67.04 1.00 11.73 B ATOM 5110 CD GLU 351 39.441 11.771 69.051 1.00 19.57 B ATOM 5111 CB TTR 352 35.06 6.678 66.391 1.00 11.72 B ATOM 5112 CB TTR 352 35.06 6.678 67.067 1.00 11.73 B ATOM 5113 CB TTR 352 35.06 6.678 67.067 1.00 11.73 B ATOM 5110 CD GLU 351 39.481 11.771 68.024 67.664 1.00 19.39 B ATOM 5110 CD GLU 351 39.481 11.771 68.024 67.664 1.00 19.39 B ATOM 5110 CD GLU 351 36.696 7.096 66.939 1.00 10.00 32.89 B ATOM 5110 CD GLU 351 36.066 7.096 66.939 1.00 10.00 32.89 B ATO											
ATOM											
15 ATOM 5099 CGZ THR 349 40.738 -3.238 63.288 1.00 17.94 B ATOM 5095 CGZ THR 349 40.738 -3.238 63.288 1.00 15.48 B ATOM 5097 O THR 349 39.992 -5.321 65.493 1.00 16.16 B ATOM 5097 O THR 349 39.992 -5.321 65.493 1.00 16.16 B ATOM 5099 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5099 CA LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5099 CA LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5100 CB LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5101 CC LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5102 CD1 LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5102 CD1 LEU 350 43.947 -9.038 62.947 1.00 11.99 B ATOM 5103 CD LEU 350 39.162 -8.172 65.567 1.00 16.48 B ATOM 5105 C LEU 350 39.162 -8.172 65.567 1.00 16.48 B ATOM 5105 C LEU 350 39.162 -8.172 65.567 1.00 16.48 B ATOM 5105 C LEU 350 39.142 -8.595 64.876 1.00 17.28 B ATOM 5105 C LEU 350 39.142 -8.595 64.876 1.00 17.28 B ATOM 5105 C LEU 350 39.142 -8.595 64.876 1.00 17.28 B ATOM 5105 C GLU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5105 C GLU 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5100 CG GLU 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5110 CD GLU 351 39.144 -9.791 69.955 1.00 26.42 B ATOM 5110 CD GLU 351 39.484 -9.791 69.955 1.00 26.42 B ATOM 5110 CD GLU 351 39.484 -9.791 69.955 1.00 22.89 B ATOM 5111 CPL GLU 351 39.484 1.11.771 69.051 1.00 29.53 B ATOM 5112 CPL GLU 351 39.484 1.11.771 69.051 1.00 29.53 B ATOM 5112 CPL GLU 351 39.484 1.11.771 69.051 1.00 29.53 B ATOM 5112 CPL GLU 351 39.484 1.11.771 69.051 1.00 29.53 B ATOM 5112 CPL GLU 351 39.484 1.11.771 69.051 1.00 29.53 B ATOM 5112 CPL GLU 351 39.486 1.11.724 69.009 1.00 32.89 B ATOM 5116 CA TTR 352 35.755 67.666 1.00 19.18 B ATOM 5112 CPL TR 352 35.755 67.966 1.00 19.97 B ATOM 5112 CPL TR 352 35.755 67.966 1.00 19.97 B ATOM 5112 CPL TR 352 35.705 -2.729 66.033 1.00 11.72 B ATOM 5112 CPL TR 352 35.705 -2.729 68.033 1.00 11.72 B ATOM 5112 CPL TR 352 35.705 -2.729 68.033 1.00 11.72 B ATOM 5120 CPL TR 352 35.705 -2.729 68.033 1.00 11.72 B ATOM 5120 CPL TR 352 35.705 -2.729 68.033 1.00 11.72 B ATOM 5120 CPL TR											
15 ATOM 50995 CCZ THR 349 39.992 -5.321 65.428 1.00 15.48 B ATOM 5096 C THR 349 39.992 -5.325 65.282 1.00 15.48 B ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5100 CB LEU 350 40.226 -7.518 64.508 1.00 15.08 B ATOM 5101 CG LEU 350 41.952 -8.496 64.206 1.00 14.08 B ATOM 5102 CD LEU 350 41.953 -8.503 62.812 1.00 10.95 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5102 CD LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5103 CD LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5103 CD LEU 350 39.162 -8.595 64.876 1.00 17.28 B ATOM 5105 C LEU 350 39.162 -8.595 64.876 1.00 17.28 B ATOM 5105 C LEU 350 39.162 -8.595 64.876 1.00 17.28 B ATOM 5107 CA GLU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5107 CA GLU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5109 CG GLU 351 38.494 -9.731 69.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.731 69.965 1.00 26.42 B ATOM 5111 CEI GLU 351 39.441 -8.866 69.003 1.00 21.84 B ATOM 5111 CEI GLU 351 38.494 -9.731 69.965 1.00 26.42 B ATOM 5113 C GLU 351 38.494 -9.731 69.965 1.00 26.42 B ATOM 5113 C GLU 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5113 C GLU 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5113 C GLU 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5113 C GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C GLU 351 37.289 -10.724 69.309 1.00 32.89 B ATOM 5117 CB TVR 352 37.368 6.756 67.646 1.00 19.57 B ATOM 5117 CB TVR 352 37.368 6.756 67.646 1.00 19.30 B ATOM 5117 CB TVR 352 37.368 6.756 67.646 1.00 19.30 B ATOM 5117 CB TVR 352 37.368 6.756 67.646 1.00 19.30 B ATOM 5117 CB TVR 352 37.568 6.756 67.943 1.00 11.72 B ATOM 5120 CEI TVR 352 35.757 66.933 1.00 11.72 B ATOM 5120 CEI TVR 352 35.757 66.933 1.00 11.72 B ATOM 5120 CEI TVR 352 35.757 66.933 1.00 11.73 B ATOM 5120 CEI TVR 352 35.757 0.2654 69.393 1.00 11.73 B ATOM 5120 CEI TVR 352 35.757 0.2654 69.393 1.00 11.73 B ATOM 5120 CEI TVR 352 35.757 0.2654 69.393 1.00 11.73 B ATOM 5120 CEI TVR 352 35.757 0	•										
ATOM 5096 C THR 349 39.992 -5.321 65.493 1.00 16.16 B ATOM 5097 O THR 349 38.770 -5.325 65.282 1.00 15.82 B ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5099 CA LEU 350 40.777 -6.339 65.157 1.00 15.00 B ATOM 5100 CB LEU 350 41.352 -8.496 64.206 1.00 14.08 B ATOM 5101 CG LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5102 CD1 LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5103 CD2 LEU 350 41.352 -8.496 64.206 1.00 10.95 B ATOM 5103 CD2 LEU 350 41.363 -8.503 62.812 1.00 10.95 B ATOM 5103 CD LEU 350 41.363 -8.595 64.876 1.00 17.28 B ATOM 5105 C LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5106 N GUJ 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5106 N GUJ 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5108 CB GUJ 351 39.144 -8.846 69.003 1.00 19.87 B ATOM 5109 CG GUJ 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5100 CD GUJ 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5110 CD GUJ 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5110 CD GUJ 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5110 CD GUJ 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5111 CD GUJ 351 39.483 -11.771 69.051 1.00 22.95 B ATOM 5112 CD2 GUJ 351 39.482 -11.716 69.403 1.00 30.21 B ATOM 5112 CD2 GUJ 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C GUJ 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5116 CA TYR 352 31.727 8.024 67.666 1.00 19.57 B ATOM 5118 CG TYR 352 31.728 9.11.724 69.309 1.00 32.89 B ATOM 5118 CG TYR 352 35.294 -1.724 60.301 1.00 19.57 B ATOM 5118 CG TYR 352 35.105 -2.729 66.331 1.00 11.72 B ATOM 5118 CG TYR 352 35.105 -2.729 66.332 1.00 11.72 B ATOM 5112 CD2 TYR 352 31.505 -2.729 66.332 1.00 11.72 B ATOM 5112 CD2 TYR 352 31.605 -2.729 66.332 1.00 11.72 B ATOM 5112 CD2 TYR 352 31.605 -2.729 66.332 1.00 11.72 B ATOM 5112 CD2 TYR 352 31.605 -2.729 66.332 1.00 11.72 B ATOM 5112 CD2 TYR 352 31.605 -2.729 66.332 1.00 11.72 B ATOM 5112 CD2 TYR 352 31.605 -2.729 66.332 1.00 11.72 B ATOM 5113 CG HIS 354 31.605 -3.584 60.305 1.00 11.72 B ATOM 5113 CG HIS 354 31.407 -1.584 60.305 1.00 11.72 B ATOM 5130 CM TYR 352 31.605 -2.729 66.332 1.00 11.72 B AT	15										
ATOM 5098 N LEU 350 40.777 -6.325 65.282 1.00 15.82 B ATOM 5098 N LEU 350 40.276 -7.518 64.508 1.00 15.00 B ATOM 5100 CG LEU 350 41.953 -8.503 62.812 1.00 10.95 B ATOM 5101 CG LEU 350 41.953 -8.503 62.812 1.00 10.81 B ATOM 5102 CD1 LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5103 CD2 LEU 350 41.963 -8.503 62.812 1.00 10.81 B ATOM 5103 CD2 LEU 350 43.147 -9.038 62.947 1.00 11.99 B ATOM 5104 C LEU 350 350 43.147 -9.038 62.947 1.00 11.99 B ATOM 5105 C LEU 350 350 38.132 -8.595 64.876 1.00 17.28 B ATOM 5105 C LEU 350 38.132 -8.595 64.876 1.00 17.28 B ATOM 5106 C LEU 351 39.443 -8.254 66.656 1.00 18.22 B ATOM 5108 CG CU 351 38.144 -8.846 69.003 1.00 19.87 B ATOM 5100 C C CU 351 39.144 -8.846 69.003 1.00 19.87 B ATOM 5110 CD CU 351 38.494 -9.791 69.965 1.00 22.642 B ATOM 5111 OZI CU 351 38.494 -9.791 69.965 1.00 22.642 B ATOM 5111 OZI CU 351 38.420 -11.196 69.403 1.00 30.21 B ATOM 5112 OZZ CU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C C CU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5116 CA TYR 352 37.68 -6.703 67.714 1.00 19.57 B ATOM 5116 CA TYR 352 37.68 -6.703 67.646 1.00 19.87 B ATOM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 19.87 B ATOM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.87 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.37 B ATOM 5120 CZ TYR 352 36.258 -5.756 69.403 1.00 19.39 B ATOM 5130 CA ATOM 5130 C	13										
20 ATOM 5098 N LEU 350 40.777 -6.339 65.157 1.00 15.00 B B ATOM 5100 CG LEU 350 41.352 -8.496 64.206 1.00 15.08 B B ATOM 5101 CG LEU 350 41.953 -8.496 64.206 1.00 10.95 B ATOM 5102 CD1 LEU 350 41.953 -8.496 64.206 1.00 10.95 B ATOM 5102 CD1 LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5103 CD2 LEU 350 42.004 -7.143 62.214 1.00 10.95 B ATOM 5103 CD2 LEU 350 39.162 -8.172 65.367 1.00 16.88 B ATOM 5105 O LEU 350 39.162 -8.172 65.367 1.00 16.88 B ATOM 5106 N GUU 351 39.462 -8.172 65.367 1.00 16.88 B ATOM 5107 CA GUU 351 39.463 -8.254 66.658 1.00 18.22 B ATOM 5108 CB GUU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5108 CB GUU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5100 CB GUU 351 39.444 -8.842 67.609 1.00 19.87 B ATOM 5100 CB GUU 351 39.444 -8.842 67.609 1.00 29.87 B ATOM 5110 CD GUU 351 39.481 -11.771 69.965 1.00 26.42 B ATOM 5110 CD GUU 351 39.481 -11.772 69.955 1.00 26.42 B ATOM 5110 CD GUU 351 39.481 -11.772 69.951 1.00 29.53 B ATOM 5111 CD GUU 351 39.481 -11.772 69.951 1.00 29.53 B ATOM 5112 CD GUU 351 37.217 -8.024 67.646 1.00 19.18 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 31.88 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 31.87 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 19.18 B ATOM 5116 CB TYR 352 37.368 -6.703 67.603 1.00 19.18 B ATOM 5116 CB TYR 352 37.368 -6.703 67.603 1.00 19.18 B ATOM 5112 CB TYR 352 36.816 -4.348 67.891 1.00 19.57 B ATOM 5112 CD TYR 352 36.816 -4.348 67.891 1.00 19.57 B ATOM 5112 CD TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5112 CD TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5122 CD TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5122 CD TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5122 CD TYR 352 35.402 -1.00 68.465 1.00 17.30 B ATOM 5123 CA ATOM 5130 CA ATOM											
20 ATOM 5109 CA LEU 350											
ATOM 5100 CB LEU 350											
ATOM 5101 CG LEU 350 41.963 -8.503 62.812 1.00 10.95 B ATOM 5103 CD1 LEU 350 42.004 -7.143 62.214 1.00 10.81 B ATOM 5103 CD2 LEU 350 39.162 -8.172 65.367 1.00 11.99 B ATOM 5105 C LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5106 N GLU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5106 N GLU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5108 CB GLU 351 39.444 -8.846 69.003 1.00 21.84 B ATOM 5109 CG GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 21.84 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 29.53 B ATOM 5112 OEZ GLU 351 37.289 -11.774 69.309 1.00 30.21 B ATOM 5112 OEZ GLU 351 37.289 -11.724 69.309 1.00 30.21 B ATOM 5113 C GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5114 O GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5116 CA TYR 352 37.368 -6.703 67.064 1.00 19.18 B ATOM 5116 CA TYR 352 37.688 -6.703 67.063 1.00 18.87 B ATOM 5118 CG TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5118 CG TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5120 CEI TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.17 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.17 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.17 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5120 CEI TYR 352 35.570 -2.654 69.282 1.00 10.05 B ATOM 5120 C ALA 353 34.684 -9.816 60.362 1.00 18.80 B ATOM 5130 C ALA 353 34.684 -9.816 60.362 1.00 1	20										
ATOM 5102 CD1 LEU 350 42.004 -7.143 62.214 1.00 10.81 B ATOM 5104 CD2 LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5105 O LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5106 N GLU 351 39.443 -8.595 64.876 1.00 17.28 B ATOM 5107 CA GLU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5108 CG GLU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5109 CG GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 22.89 B ATOM 5111 OZI GLU 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 OZI GLU 351 37.227 -8.024 67.664 1.00 19.18 B ATOM 5113 C GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5114 O GLU 351 36.126 -8.569 67.714 1.00 19.57 B ATOM 5115 N TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 36.258 -5.756 67.644 1.00 17.30 B ATOM 5117 CB TYR 352 36.258 -5.756 67.601 1.00 14.25 B ATOM 5119 CD1 TYR 352 35.105 -2.729 66.933 1.00 11.26 B ATOM 5120 CEI TYR 352 36.258 -5.756 67.891 1.00 14.25 B ATOM 5120 CEI TYR 352 36.258 -5.766 67.891 1.00 14.25 B ATOM 5120 CEI TYR 352 36.264 -5.729 66.933 1.00 11.26 B ATOM 5120 CEI TYR 352 36.264 -5.729 66.933 1.00 11.26 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.077 1.00 11.73 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 14.25 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 14.25 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 11.26 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 11.26 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 11.26 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 CEI TYR 352 36.264 -5.896 67.891 1.00 10.15 B ATOM 5120 C ALA 353 36.15 -5.926 66.497 1.00	20										
25 ATOM 5103 CDZ LEU 350 39.162 -8.172 65.367 1.00 11.99 B ATOM 5106 N C LEU 350 39.162 -8.172 65.367 1.00 16.48 B ATOM 5106 N GLU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5106 N GLU 351 39.443 -8.254 66.658 1.00 18.22 B ATOM 5108 CB GLU 351 39.444 -8.846 69.003 1.00 21.84 B ATOM 5108 CB GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 22.88 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 22.89 B ATOM 5112 OEZ GLU 351 37.289 -11.724 69.309 1.00 30.21 B ATOM 5112 OEZ GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5114 O GLU 351 37.289 -11.724 69.309 1.00 19.57 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5117 CB TYR 352 36.816 -4.348 67.891 1.00 19.57 B ATOM 5118 CG TYR 352 36.816 -4.348 67.891 1.00 14.25 B ATOM 5119 CDI TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5120 CEL TYR 352 34.699 -1.584 69.803 1.00 11.72 B ATOM 5121 CDZ TYR 352 34.699 -1.584 69.831 1.00 10.15 B ATOM 5122 CDZ TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5123 CZ TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5126 O TYR 352 34.210 -1.078 68.322 1.00 10.15 B ATOM 5127 CDZ TYR 352 34.699 -1.584 69.433 1.00 10.15 B ATOM 5128 CA ALA 353 35.402 -5.814 66.362 1.00 18.80 B ATOM 5128 CA ALA 353 35.402 -5.814 66.362 1.00 18.80 B ATOM 5128 CA ALA 353 35.402 -5.814 66.362 1.00 18.33 B ATOM 5130 C ALA 353 35.402 -7.249 63.365 1.00 18.36 B ATOM 5131 O ALA 353 35.402 -7.249 63.365 1.00 18.36 B ATOM 5131 CA ALA 353 35.402 -7.229 66.931 1.00 19.93 B ATOM 5130 C ALA 353 35.402 -5.814 66.302 1.00 18.30 B ATOM 5130 C ALA 353 35.402 -5.814 66.302 1.00 18.30 B ATOM 5130 C ALA 353 35.402 -5.891 63.951 1.00 17.31 B ATOM 5130 CA ALA 353 35.402 -5.891 63.951 1.00 18.30 B ATOM 5130 CA ALA 353 35.402 -5.891 63.951 1.00 18.30 B ATOM 5130 CA ALA 353 35.402 -5.891 63.951 1.00 18.30 B ATOM 5130 CA ALA 353 35.402 -5.891 63.951 1.00 18.30 B ATOM 5140 CA BLS ALS ALS ALS ALS ALS ALS ALS ALS ALS A											
25 AROM 5104 C LEU 350 39.162 -8.172 65.367 1.00 16.48 B AROM 5105 O LEU 350 39.162 -8.172 65.367 1.00 17.28 B AROM 5106 N GLU 351 38.132 -8.595 64.876 1.00 17.28 B AROM 5107 CA GLU 351 38.132 -8.254 66.658 1.00 18.22 B AROM 5109 CG GLU 351 38.494 -9.791 69.965 1.00 21.84 B AROM 5109 CG GLU 351 38.494 -9.791 69.965 1.00 22.89 B AROM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 22.89 B AROM 5111 OEI GLU 351 39.481 -11.771 69.051 1.00 29.53 B AROM 5112 OEZ GLU 351 37.289 -11.724 69.309 1.00 32.89 B AROM 5113 C GLU 351 37.289 -11.724 69.309 1.00 19.18 B AROM 5113 C GLU 351 37.289 -11.724 69.309 1.00 19.57 B AROM 5115 N TYR 352 37.368 -6.703 67.603 1.00 18.87 B AROM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 19.18 B AROM 5117 CB TYR 352 36.258 -5.756 67.646 1.00 17.30 B AROM 5119 CD TYR 352 35.105 -2.729 66.933 1.00 11.25 B AROM 5119 CD TYR 352 35.105 -2.729 66.933 1.00 11.26 B AROM 5120 CEI TYR 352 34.220 -1.649 67.067 1.00 11.25 B AROM 5120 CEI TYR 352 34.220 -1.649 67.067 1.00 11.17 B AROM 5120 CEI TYR 352 34.024 -1.078 68.232 1.00 11.26 B AROM 5124 OH TYR 352 35.794 -3.239 68.039 1.00 11.26 B AROM 5126 C TYR 352 35.570 -2.654 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 CEI TYR 352 35.795 -6.694 69.282 1.00 10.15 B AROM 5120 C ALA 353 34.227 -7.249 66.993 1.00											
ATOM 5105 O LEU 350 38.132 -8.595 64.876 1.00 17.28 B ATOM 5107 CA GLU 351 39.443 -8.254 66.658 1.00 19.87 B ATOM 5108 CB GLU 351 39.144 -8.846 65.003 1.00 19.87 B ATOM 5108 CB GLU 351 38.514 -8.842 67.609 1.00 19.87 B ATOM 5100 CG GLU 351 38.494 -9.791 65.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 65.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 69.051 1.00 29.53 B ATOM 5112 OE2 GLU 351 37.289 -11.724 69.309 1.00 29.53 B ATOM 5112 OE2 GLU 351 37.289 -11.724 69.309 1.00 29.53 B ATOM 5114 O GLU 351 37.217 -8.024 67.646 1.00 19.18 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CG TYR 352 35.994 -3.299 66.993 1.00 11.72 B ATOM 5118 CG TYR 352 35.994 -3.299 66.993 1.00 11.72 B ATOM 5119 CD1 TYR 352 35.105 -2.729 66.993 1.00 11.72 B ATOM 5120 CE1 TYR 352 35.105 -2.729 66.993 1.00 11.72 B ATOM 5120 CE1 TYR 352 35.5794 -2.654 69.282 1.00 10.17 B ATOM 5123 CZ TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 35.795 -2.654 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 35.795 -2.654 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 35.795 -2.654 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 35.795 -2.654 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 35.795 -2.654 69.282 1.00 10.15 B ATOM 5125 CT TYR 352 35.795 -2.654 69.282 1.00 10.15 B ATOM 5126 CT TYR 352 35.795 -2.654 69.282 1.00 10.15 B ATOM 5126 CT TYR 352 35.795 -2.554 66.935 1.00 27.75 B ATOM 5126 CT TYR 352 33.17											
ATOM 5106 N GLU 351 39.443 -8.254 66.558 1.00 18.22 B ATOM 5107 CA GLU 351 39.144 -8.846 69.003 1.00 19.87 B ATOM 5108 CB GLU 351 39.144 -8.846 69.003 1.00 21.84 B ATOM 5109 CG GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5111 OEI GLU 351 38.494 -9.791 69.965 1.00 30.21 B ATOM 5112 OE2 GLU 351 37.289 -11.724 69.051 1.00 22.89 B ATOM 5113 C GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C GLU 351 37.287 -11.724 69.309 1.00 32.89 B ATOM 5113 C GLU 351 37.287 -11.724 69.309 1.00 19.57 B ATOM 5115 N TYR 352 36.258 -6.756 67.646 1.00 19.18 B ATOM 5116 CA TYR 352 36.816 -8.559 67.714 1.00 19.57 B ATOM 5116 CA TYR 352 36.816 -4.348 67.646 1.00 19.25 B ATOM 5118 CG TYR 352 36.816 -4.348 67.891 1.00 14.25 B ATOM 5119 CDI TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5120 CEI TYR 352 36.258 -5.756 67.663 1.00 14.25 B ATOM 5120 CEI TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5120 CEI TYR 352 36.256 -2.729 66.933 1.00 11.26 B ATOM 5120 CEI TYR 352 35.950 -2.654 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5120 CT TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5120 CT TYR 352 34.699 -1.584 69.431 1.00 19.39 B ATOM 5127 N ALA 353 36.155 -5.822 65.216 1.00 18.80 B ATOM 5127 N ALA 353 36.354 -5.891 63.951 1.00 17.31 B ATOM 5120 CA ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 36.359 -5.698 62.821 1.00 18.30 B ATOM 5131 C HIS 354 35.314 -7.29 9.661 63.994 1.00 22.75 B ATOM 5132 CR BALA 353 36.359 -5.891 63.951 1.00 17.31 B ATOM 5134 CB HIS 354 35.314 -7.221 63.855 1.00 25.34 B ATOM 5137 NDI HIS 354 35.314 -7.221 63.855 1.00 25.34 B ATOM 5136 CD HIS 354 35.314 -7.221 63.855 1.00 22.75 B ATOM 5137 CR HIS 354 35.314 -7.221 63.855 1.00 22.75 B ATOM 5136 CD HIS 354 35.314 -7.221 63.855 1.00 22.75 B ATOM 5137 CR HIS 354 35.317 -7.225 63.053 1.00 22.75 B ATOM 5137 CR HIS 354 35.317 -7.852 66.891 1.00 20.90 B ATOM 5137 NDI HIS 354 35.317 -7.225 63.053 1.00 22.76 B ATOM 5136 CD ARG 355 31.055 -9.255 66.891 1.00 20.70 B ATOM 5137 CR HIS 354 35.317 -7.225 63.053 1.00 22.76 B ATO	25										
ATOM 5107 CA GLU 351 38.514 -8.846 57.609 1.00 19.87 B ATOM 5109 CG GLU 351 38.494 -9.791 69.965 1.00 21.84 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5110 CD GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5111 CDEI GLU 351 38.494 -9.791 69.965 1.00 26.42 B ATOM 5112 OE2 GLU 351 37.289 -11.774 69.051 1.00 29.53 B ATOM 5112 OE2 GLU 351 37.289 -11.774 69.309 1.00 29.53 B ATOM 5114 O GLU 351 37.289 -11.774 69.309 1.00 29.53 B ATOM 5115 N TYR 352 37.269 -11.724 69.309 1.00 19.18 B ATOM 5116 CA TYR 352 37.368 -6.703 67.646 1.00 19.18 B ATOM 5116 CA TYR 352 36.816 -4.348 67.603 1.00 19.18 B ATOM 5117 CB TYR 352 36.816 -4.348 67.603 1.00 11.72 B ATOM 5118 CG TYR 352 35.794 -3.229 66.933 1.00 11.72 B ATOM 5119 CDI TYR 352 35.794 -3.229 66.933 1.00 11.72 B ATOM 5120 CEI TYR 352 35.794 -3.229 66.933 1.00 11.72 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5124 OH TYR 352 33.1756 09.186 49.33 1.00 9.37 B ATOM 5125 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5126 OH TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5126 OH TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5127 CB ALA 353 35.406 -5.891 63.991 1.00 12.75 B ATOM 5128 CA ALA 353 35.406 -5.891 63.991 1.00 12.75 B ATOM 5128 CA ALA 353 35.406 -5.891 63.991 1.00 12.75 B ATOM 5127 CB ALA 353 35.406 -5.891 63.991 1.00 12.75 B ATOM 5130 C ALA 353 35.406 -5.891 63.991 1.00 18.80 B ATOM 5131 CA ALB 353 35.406 -5.891 63.991 1.00 18.33 B ATOM 5132 CA BLA 353 35.406 -5.891 63.991 1.00 18.30 B ATOM 5134 CB HIS 354 35.316 -4.297 -9.661 63.994 1.00 18.30 B ATOM 5137 CB ALA 353 35.406 -7.221 63.785 1.00 18.30 B ATOM 5137 CB ALA 353 35.406 -7.221 63.785 1.00 18.30 B ATOM 5137 CB ALA 353 35.406 -7.221 63.785 1.00 18.30 B ATOM 5138 CB ALA 353 35.406 -7.221 63.785 1.00 18.30 B ATOM 5137 CB ALA 353 35.406 -7.221 63.785 1.00 18.30 B ATOM 5138 CB ALB 353 35.406 -7.221 63.785 1.00 18.30 B ATOM 5137 CB ALB 353 35.406 -7.221 63.785 1.00 18.50 B ATOM 5137 CB ALB 353 35.406 -7.221 63.785 1.00 18.50	23		_								
ATOM \$108 CB GLU 351 39:144 -8.846 69:003 1.00 26:42 B											
30 ATOM 5109 CG GLU 351 38.494 -9.791 69.965 1.00 26.42 8 ATOM 5111 OCD GLU 351 38.494 -9.791 69.965 1.00 30.21 8 ATOM 5112 OCE GLU 351 39.481 -11.771 69.051 1.00 29.53 8 ATOM 5113 C GLU 351 37.289 -11.774 69.309 1.00 32.25 89 ATOM 5114 O GLU 351 37.289 -11.774 69.309 1.00 32.89 8 ATOM 5115 N TYR 352 36.126 -8.569 67.714 1.00 19.57 8 ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 18.87 8 ATOM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 17.30 8 ATOM 5117 CB TYR 352 36.8616 -4.348 67.891 1.00 11.73 8 ATOM 5119 CD TYR 352 35.105 -2.729 66.933 1.00 11.72 8 ATOM 5120 CEI TYR 352 34.220 -1.649 67.067 1.00 11.17 8 ATOM 5121 CD2 TYR 352 34.290 -1.649 67.067 1.00 11.17 8 ATOM 5122 CEZ TYR 352 34.290 -1.649 69.433 1.00 10.15 8 ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 10.15 8 ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 11.62 8 ATOM 5126 C TYR 352 33.175 0.010 68.445 1.00 14.22 8 ATOM 5126 C TYR 352 35.144 -5.814 66.362 1.00 18.80 8 ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.80 8 ATOM 5130 C ALA 353 36.155 -5.891 63.991 1.00 17.31 8 ATOM 5131 C ALA 353 36.155 -5.891 63.991 1.00 17.31 8 ATOM 5131 C ALA 353 36.156 -5.891 63.991 1.00 10.15 8.8 ATOM 5123 C TYR 352 33.175 0.010 68.445 1.00 14.22 8 ATOM 5126 C TYR 352 33.175 0.010 68.455 1.00 18.30 8 ATOM 5127 N ALA 353 36.115 -5.892 66.407 1.00 19.93 8 ATOM 5130 C ALA 353 36.115 -5.892 66.407 1.00 19.93 8 ATOM 5131 C ALA 353 36.156 -5.891 63.991 1.00 17.31 8 ATOM 5131 C ALA 353 36.156 -5.891 63.991 1.00 17.31 8 ATOM 5132 C THR 354 34.217 -5.869 62.821 1.00 16.39 8 ATOM 5133 C ALA 353 36.156 -5.891 63.991 1.00 20.34 8 ATOM 5134 C B ALA 353 36.156 -5.891 63.991 1.00 20.34 8 ATOM 5135 C G HIS 354 34.779 -9.661 63.994 1.00 20.34 8 ATOM 5136 C B ALA 353 36.156 -5.891 63.991 1.00 20.34 8 ATOM 5136 C B ALA 353 36.40 -7.221 64.509 1.00 22.75 8 ATOM 5136 C B ALS 354 34.779 -9.661 63.994 1.00 20.34 8 ATOM 5136 C B ALS 354 34.779 -9.661 63.994 1.00 20.27 8 ATOM 5136 C B ALS 354 34.797 -13.01 65.569 1.00 20.27 8 ATOM 5137 C B ALS 355 31.177 -8.826 66.407 1.00 20.03 8 ATOM 5138											B
30 ATOM 5110 CD GLU 351 38.420 -11.196 69.403 1.00 30.21 B ATOM 5111 OEI GLU 351 37.289 -11.771 69.051 1.00 29.53 B ATOM 5112 OE2 GLU 351 37.289 -11.772 69.051 1.00 29.53 B ATOM 5113 C GLU 351 37.289 -11.772 69.051 1.00 32.89 B ATOM 5114 O GLU 351 37.289 -11.772 69.050 1.00 32.89 B ATOM 5115 N TYR 352 36.26 -8.559 67.714 1.00 19.57 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 36.816 -4.348 67.891 1.00 14.25 B ATOM 5117 CB TYR 352 35.056 -2.729 66.933 1.00 17.30 B ATOM 5118 CG TYR 352 35.05 -2.729 66.933 1.00 11.72 B ATOM 5119 CD1 TYR 352 35.05 -2.729 66.933 1.00 11.26 B ATOM 5120 CEI TYR 352 35.05 -2.729 66.933 1.00 11.26 B ATOM 5121 CD2 TYR 352 35.05 -2.729 66.933 1.00 11.26 B ATOM 5122 CE2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5123 CZ TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5124 ON TYR 352 33.15 70 -2.654 69.433 1.00 9.37 B ATOM 5125 C TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5126 O TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5127 N ALA 353 36.115 -5.822 66.407 1.00 18.33 B ATOM 5128 CA ALA 353 35.406 -5.824 66.907 1.00 19.93 B ATOM 5129 CB ALA 353 35.406 -5.824 66.907 1.00 18.33 B ATOM 5130 C ALA 353 35.406 -5.825 66.407 1.00 18.33 B ATOM 5131 O ALA 353 35.406 -5.822 66.407 1.00 18.30 B ATOM 5132 N HIS 354 35.354 -2.224 63.785 1.00 18.36 B ATOM 5133 CA ALA 353 35.406 -5.821 63.951 1.00 17.31 B ATOM 5134 CB HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5135 CG HIS 354 35.354 -8.319 64.19 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.354 -8.319 64.19 1.00 22.75 B ATOM 5137 ND1 HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5138 CEI HIS 354 34.877 -9.286 66.497 1.00 22.75 B ATOM 5136 CD2 ARG 355 32.370 -9.285 66.891 1.00 22.75 B ATOM 5137 ND1 HIS 354 34.977 -13.016 63.052 1.00 18.53 B ATOM 5140 C HIS 354 34.897 -13.016 63.052 1.00 22.75 B ATOM 5140 C ARG 355 32.370 -9.285 66.891 1.00 22.76 B ATOM 5140 C ARG 355 30.802 -8.942 72.281 1.00 31.17 B ATOM 5140 C ARG 355 30.040 -8.992 66.6453 1.00 23.15 B											В
ATOM 5111 ORI GLU 351 39.481 -11.771 69.051 1.00 29.53 B ATOM 5112 OR2 GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C GLU 351 37.217 -8.024 67.646 1.00 19.18 B ATOM 5115 N TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5117 CB TYR 352 36.816 -4.348 67.891 1.00 11.73 B ATOM 5118 CG TYR 352 36.816 -4.348 67.891 1.00 11.72 B ATOM 5119 CD1 TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5120 CE1 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5121 CD2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5122 CE2 TYR 352 34.290 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 10.15 B ATOM 5124 CN TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 O TYR 352 35.44 -3.09 68.392 1.00 11.62 B ATOM 5127 N ALA 353 36.115 -5.822 66.407 1.00 19.33 B ATOM 5128 CA ALA 353 36.115 -5.822 65.216 1.00 18.80 B ATOM 5129 CB ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 10.16.39 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 10.16.39 B ATOM 5132 C B ALA 353 36.406 -5.891 63.951 1.00 19.33 B ATOM 5133 CA ALA 353 36.406 -5.891 63.951 1.00 17.31 B ATOM 5134 CB HIS 354 35.761 -10.712 64.599 1.00 22.75 B ATOM 5135 CG HIS 354 34.779 -9.661 63.994 1.00 22.75 B ATOM 5134 CB HIS 354 35.761 -10.712 64.599 1.00 22.75 B ATOM 5135 CG HIS 354 34.779 -9.661 63.994 1.00 22.75 B ATOM 5137 NDI HIS 354 35.761 -10.712 64.599 1.00 22.75 B ATOM 5138 CE1 HIS 354 34.5761 -10.712 64.599 1.00 22.75 B ATOM 5137 NDI HIS 354 35.5161 -10.712 64.599 1.00 22.75 B ATOM 5134 CB HIS 354 34.511 -14.62 64.427 1.00 26.03 B ATOM 5134 CB HIS 354 34.511 -14.62 64.927 1.00 22.75 B ATOM 5134 CB HIS 354 34.511 -14.62 64.927 1.00 22.75 B ATOM 5137 NDI HIS 354 35.516 -7.221 64.929 1.00 22.75 B ATOM 5138 CC HIS 354 34.511 -14.62 64.927 1.00 22.75 B ATOM 5137 NDI HIS 354 35.510 -7.221 68.239 1.00 20.70 B ATOM 5140 C HIS 354 34.511 -14.62 64.927 1.00 20.23 B ATOM 5140 C HIS 354 34.511 -14.62 64.927 1.00 20.20 B ATOM 5147 ND ALA 355 31.60 -9.811 64.796 1.00 20.2	20		5109	CG	GLU	351	38.494	-9.791	69.965	1.00 26.42	В
ATOM 5112 OE2 GLU 351 37.289 -11.724 69.309 1.00 32.89 B ATOM 5113 C GLU 351 37.217 -8.024 67.646 1.00 19.18 B ATOM 5114 O GLU 351 36.126 -8.569 67.714 1.00 19.57 B ATOM 5115 N TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5117 CB TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5118 CG TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5119 CD1 TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5119 CD1 TYR 352 36.258 -5.756 67.646 1.00 11.72 B ATOM 5120 CE1 TYR 352 36.258 -5.756 67.646 1.00 11.72 B ATOM 5120 CE1 TYR 352 36.810 -4.348 67.891 1.00 14.25 B ATOM 5120 CE1 TYR 352 35.794 -3.239 66.393 1.00 11.72 B ATOM 5121 CD2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5122 CE2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5122 CE2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 10.15 B ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5125 C TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5126 C TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5127 N ALA 353 36.115 -5.822 66.407 1.00 19.93 B ATOM 5128 CA ALA 353 36.115 -5.822 65.216 1.00 18.80 B ATOM 5129 CB ALA 353 36.315 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5130 C ALA 353 36.406 -5.891 63.951 1.00 17.31 B ATOM 5131 CA ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 CA ALA 353 36.406 -9.961 63.994 1.00 20.34 B ATOM 5131 CA ALA 353 36.407 -9.661 63.994 1.00 20.34 B ATOM 5131 CA BHIS 354 35.302 -12.121 64.509 1.00 25.37 B ATOM 5134 CB HIS 354 35.302 -12.211 64.294 1.00 25.37 B ATOM 5134 CB HIS 354 35.302 -12.212 66.407 1.00 19.39 B ATOM 5136 CD HIS 354 35.302 -12.211 64.294 1.00 25.34 B ATOM 5131 CA ARG 355 33.486 -9.811 64.199 1.00 20.23 B ATOM 5134 CB HIS 354 35.302 -12.211 64.294 1.00 25.34 B ATOM 5134 CB HIS 354 35.302 -12.211 64.294 1.00 25.37 B ATOM 5136 CD ARG 355 33.486 -9.811 64.796 1.00 20.23 B ATOM 5140 CD HIS 354 35.31 -12.725 63.053 1.00 22.75 B ATOM 5141 O HIS 354 32.512 -10.417 64.509 1.00 20.70 B ATOM	30	MOTA	5110	CD	GLU	351	38.420	-11.196	69.403	1.00 30.21	В
ATOM 5113 C GLU 351 37.217 -8.024 67.646 1.00 19.18 B ATOM 5114 O GLU 351 36.126 -8.569 67.714 1.00 19.57 B ATOM 5115 N TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5117 CB TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5118 CG TYR 352 35.794 -3.239 68.039 1.00 11.26 B ATOM 5119 CDI TYR 352 35.105 -2.729 66.933 1.00 11.26 B ATOM 5120 CEI TYR 352 35.500 -2.654 69.282 1.00 10.15 B ATOM 5121 CD2 TYR 352 34.202 -1.649 67.067 1.00 11.17 B ATOM 5123 CZ TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5124 CH TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5125 C TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 C TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.80 B ATOM 5128 CA ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 36.156 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 36.156 -5.822 65.216 1.00 18.33 B ATOM 5120 C ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 33.542 -7.249 63.365 1.00 18.36 B ATOM 5131 C ALA 353 33.5542 -7.249 63.365 1.00 18.36 B ATOM 5131 C ALA 353 33.5542 -7.221 63.785 1.00 18.36 B ATOM 5131 C ALA 353 33.5542 -7.221 63.685 1.00 18.36 B ATOM 5131 C ALA 353 33.542 -7.221 63.695 1.00 22.75 B ATOM 5131 C ALA 353 33.5542 -7.2249 63.365 1.00 25.34 B ATOM 5131 C ALA 353 33.542 -7.2249 63.365 1.00 25.34 B ATOM 5131 C ALA 353 33.546 -7.221 63.785 1.00 25.34 B ATOM 5134 C ALA 353 33.543 -7.2249 63.		MOTA	5111	OE1	GLU	351	39.481	-11.771	69.051	1.00 29.53	В
35 ATOM 5114 O GLU 351 36.126 -8.569 67.714 1.00 19.57 B ATOM 5115 N TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 36.258 -5.756 67.604 1.00 17.30 B ATOM 5117 CB TYR 352 36.816 -4.348 67.891 1.00 14.25 B ATOM 5118 CG TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5119 CD1 TYR 352 35.105 -2.729 66.933 1.00 11.26 B ATOM 5120 CE1 TYR 352 35.105 -2.729 66.933 1.00 11.26 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CE2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5122 CE2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5122 CE2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.699 -1.584 69.433 1.00 11.62 B ATOM 5125 C TYR 352 34.175 0.010 68.445 1.00 14.22 B ATOM 5126 O TYR 352 34.175 0.010 68.445 1.00 14.22 B ATOM 5126 C TYR 352 34.274 -5.852 66.407 1.00 11.62 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.80 B ATOM 5128 CA ALA 353 36.115 -5.822 66.407 1.00 19.93 B ATOM 5128 CA ALA 353 36.315 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 17.31 B ATOM 5130 C ALA 353 36.359 -5.698 62.821 1.00 17.31 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5132 N HIS 354 35.344 -7.224 63.365 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5130 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5130 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5134 CB HIS 354 35.311 -12.725 63.959 1.00 22.75 B ATOM 5140 CB HIS 354 35.311 -12.725 63.959 1.00 22.75 B ATOM 5140 CB HIS 354 36.979 -9.651 63.999 1.00 22.75 B ATOM 5140 CB HIS 354 36.9		MOTA	5112	OE2	GLU	351	37.289	-11.724	69.309	1.00 32.89	В
35 ATOM 5115 N TYR 352 37.368 -6.703 67.603 1.00 18.87 B ATOM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5117 CB TYR 352 36.816 -4.348 67.891 1.00 14.25 B ATOM 5118 CG TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5119 CD1 TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5120 CE1 TYR 352 35.05 -2.729 66.933 1.00 11.17 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CE2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CE2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5124 CD TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5125 C TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 C TYR 352 35.544 2-5.814 66.362 1.00 18.80 B ATOM 5126 C TYR 352 35.406 -5.891 63.951 1.00 17.31 B ATOM 5128 CA ALA 353 36.115 -5.822 66.407 1.00 19.93 B ATOM 5129 CB ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 36.355 -5.698 62.821 1.00 16.39 B ATOM 5129 CB ALA 353 36.355 -5.698 62.821 1.00 16.39 B ATOM 5132 N HIS 354 34.680 -7.221 63.785 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -7.249 63.365 1.00 18.10 B ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5135 CG HIS 354 34.779 -9.661 63.994 1.00 22.75 B ATOM 5137 CD HIS 354 34.779 -9.661 63.994 1.00 22.75 B ATOM 5137 CD HIS 354 34.779 -9.661 63.994 1.00 25.577 B ATOM 5137 CD HIS 354 34.779 -9.661 63.994 1.00 25.577 B ATOM 5137 CD HIS 354 34.779 -9.661 63.994 1.00 25.577 B ATOM 5134 CD HIS 354 34.797 -13.031 65.156 1.00 25.577 B ATOM 5134 CD HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 34.511 -14.162 64.994 1.00 20.70 B ATOM 5140 C HIS 354 34.511 -14.162 64.994 1.00 20.70 B ATOM 5140 C HIS 354 34.511 -14.162 64.994 1.00 20.70 B ATOM 5140 C HIS 354 34.511 -14.162 64.994 1.00 20.70 B ATOM 5140 C HIS 354 34.511 -14.162 64.994 1.00 20.70 B ATOM 5140 C HIS 354 34.511 -14.162 64.994 1.00 20.70 B ATOM 5140 C HIS 354 34.511 -14.162 64.994 1.00 20.70 B ATOM	•	ATOM	5113	C	GLU	351	37.217	-8.024	67.646	1.00 19.18	В
ATOM 5116 CA TYR 352 36.216 -4.348 67.891 1.00 17.30 B ATOM 5117 CB TYR 352 35.816 -4.348 67.891 1.00 14.25 B ATOM 5118 CG TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5119 CD1 TYR 352 35.794 -3.239 66.933 1.00 11.72 B ATOM 5120 CE1 TYR 352 35.105 -2.729 66.933 1.00 11.26 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CCZ TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CCZ TYR 352 34.024 -1.078 68.322 1.00 10.15 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 C TYR 352 34.21 -5.814 66.362 1.00 18.80 B ATOM 5127 N ALA 353 35.442 -5.814 66.362 1.00 18.80 B ATOM 5128 CA ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.155 -5.822 65.216 1.00 18.33 B ATOM 5130 C ALA 353 36.155 -5.698 62.281 1.00 17.31 B ATOM 5131 O ALA 353 33.5406 -5.891 63.951 1.00 18.36 B ATOM 5131 O ALA 353 33.5406 -7.221 63.785 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5134 CB HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5135 CG HIS 354 35.302 -7.249 63.365 1.00 25.34 B ATOM 5136 CD HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5137 NDI HIS 354 34.779 -9.661 63.994 1.00 25.34 B ATOM 5138 CE1 HIS 354 35.302 -12.21 64.294 1.00 25.34 B ATOM 5136 CD HIS 354 35.31 -12.725 63.053 1.00 25.77 B ATOM 5137 NDI HIS 354 34.797 -13.031 65.156 1.00 25.34 B ATOM 5138 CE1 HIS 354 34.797 -13.031 65.156 1.00 25.34 B ATOM 5136 CD HIS 354 35.311 -12.725 63.053 1.00 27.7 B ATOM 5137 NDI HIS 354 34.797 -13.031 65.156 1.00 20.27 B ATOM 5140 C HIS 354 35.302 -12.21 64.294 1.00 25.34 B ATOM 5140 C HIS 354 35.302 -12.21 64.294 1.00 25.34 B ATOM 5140 C HIS 354 35.302 -12.21 64.294 1.00 25.34 B ATOM 5140 C HIS 354 35.302 -12.21 64.294 1.00 25.34 B ATOM 5140 C HIS 354 35.302 -12.21 64.294 1.00 20.00 2.70 B ATOM 5140 C HIS 354 34.797 -38.66 69.339 1.00 20.70 B ATOM 5140 C HIS 354 34.797 -8.516 60.00 70.00 20.70 B ATOM 5140 C HIS 354 36.600 60.00 70.00 70.00 18.53 B ATOM 5140 C HIS 354 36.00 70.00 70.00 70.00 18.53 B ATOM 5140		MOTA	5114	0	GLU	351	36.126	-8.569	67.714	1.00 19.57	В
ATOM 5116 CA TYR 352 36.258 -5.756 67.646 1.00 17.30 B ATOM 5117 CB TYR 352 36.816 -4.348 67.891 1.00 14.25 B ATOM 5118 CG TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5119 CD1 TYR 352 35.105 -2.729 66.933 1.00 11.72 B ATOM 5120 CE1 TYR 352 35.105 -2.654 69.282 1.00 10.15 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CC2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.624 -1.078 68.322 1.00 11.62 B ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 C TYR 352 34.21 -5.814 66.362 1.00 18.80 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.359 -5.698 62.281 1.00 17.31 B ATOM 5131 C ALA 353 36.359 -5.698 62.281 1.00 16.39 B ATOM 5131 O ALA 353 33.5406 -5.891 63.951 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CB HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5134 CB HIS 354 35.302 -7.249 63.365 1.00 18.10 B ATOM 5135 CG HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5137 NDI HIS 354 35.31 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5134 CB HIS 354 35.31 -12.725 63.053 1.00 25.77 B ATOM 5134 CB HIS 354 34.797 -13.031 65.156 1.00 25.34 B ATOM 5136 CD HIS 354 35.31 -12.725 63.053 1.00 25.77 B ATOM 5137 NDI HIS 354 35.31 -12.725 63.053 1.00 20.70 B ATOM 5140 C HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5140 C HIS 354 35.302 -9.255 66.995 1.00 20.70 B ATOM 5147 N R ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5147 N R ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5148 CZ ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5148 CZ ARG 355 32.837 -9.255 66.995 1.00 20.76 B ATOM 5148 CZ ARG 355 32.802 -8.721 68.239 1.00 20.70 B ATOM 5148 CZ ARG 355 30.000 -8.942 72.281 1.00 31.26 B ATOM 5148 CZ ARG 355 30.000 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 30.000 -8.942 72.281 1.00 31.26 B ATOM 5	35	MOTA	.5115	N	TYR	352	37.368		67.603		
## ATOM 5117 CB TYR 352 35.816 -4.348 67.891 1.00 14.25 B ## ATOM 5119 CD1 TYR 352 35.105 -2.729 68.039 1.00 11.72 B ## ATOM 5120 CE1 TYR 352 35.105 -2.729 66.933 1.00 11.26 B ## ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ## ATOM 5122 CE2 TYR 352 34.699 -1.584 69.282 1.00 10.15 B ## ATOM 5123 CZ TYR 352 34.699 -1.584 69.282 1.00 10.15 B ## ATOM 5124 CH TYR 352 34.699 -1.584 69.282 1.00 10.15 B ## ATOM 5125 CZ TYR 352 34.699 -1.584 69.282 1.00 11.62 B ## ATOM 5125 CZ TYR 352 34.699 -1.584 69.282 1.00 11.62 B ## ATOM 5126 CZ TYR 352 34.699 -1.584 69.282 1.00 11.62 B ## ATOM 5125 CZ TYR 352 34.699 -1.584 69.282 1.00 11.62 B ## ATOM 5126 C TYR 352 34.024 -1.078 68.322 1.00 14.22 B ## ATOM 5125 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ## ATOM 5126 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ## ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ## ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ## ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ## ATOM 5131 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ## ATOM 5132 N HIS 354 35.544 -8.319 64.119 1.00 19.39 B ## ATOM 5133 CA HIS 354 34.779 -9.661 64.199 1.00 25.34 B ## ATOM 5136 CD2 HIS 354 34.779 -9.661 64.294 1.00 25.34 B ## ATOM 5138 CE1 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ## ATOM 5138 CE1 HIS 354 34.81 -13.948 63.164 1.00 20.23 B ## ATOM 5138 CE1 HIS 354 34.81 -13.948 63.164 1.00 20.23 B ## ATOM 5140 C HIS 354 34.81 -13.948 63.164 1.00 20.23 B ## ATOM 5140 C HIS 354 33.860 -9.811 64.796 1.00 20.24 B ## ATOM 5140 C		ATOM	5116	CA	TYR						
40 ATOM 5118 CG TYR 352 35.794 -3.239 68.039 1.00 11.72 B ATOM 5120 CE1 TYR 352 35.105 -2.729 66.933 1.00 11.26 B ATOM 5121 CD2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5122 CE2 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5122 CE2 TYR 352 34.699 -1.584 69.282 1.00 10.15 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 11.62 B ATOM 5125 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5126 O TYR 352 34.217 -5.852 66.07 1.00 19.93 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.10 B ATOM 5131 O ALA 353 35.468 -7.221 63.785 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -7.249 63.365 1.00 18.10 B ATOM 5134 CB HIS 354 34.779 -9.661 63.994 1.00 22.75 B ATOM 5135 CG HIS 354 34.797 -13.031 65.156 1.00 22.75 B ATOM 5136 CD2 HIS 354 34.891 -1.725 63.053 1.00 22.75 B ATOM 5137 ND1 HIS 354 34.891 -1.725 63.053 1.00 22.75 B ATOM 5138 CE1 HIS 354 34.891 -1.3.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.891 -1.3.948 63.164 1.00 26.03 B ATOM 5130 C HIS 354 34.891 -1.3.948 63.164 1.00 26.03 B ATOM 5130 C HIS 354 34.891 -1.3.948 63.164 1.00 26.03 B ATOM 5130 C HIS 354 34.891 -1.3.948 63.164 1.00 26.03 B ATOM 5134 CB HIS 354 34.891 -1.3.948 63.164 1.00 26.03 B ATOM 5140 C HIS 354 34.891 -1.3.948 63.164 1.00 26.07 B ATOM 5140 C HIS 354 34.891 -1.725 63.053 1.00 22.77 B ATOM 5142 CB ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5144 CB ARG 355 32.833 -8.721 68.239 1.00 22.76 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.12 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.55 B		ATOM	5117	CB							
40 ATOM 5119 CD1 TYR 352 35.105 -2.729 66.933 1.00 11.26 B ATOM 5120 CE1 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5121 CD2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5122 CE2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5124 OH TYR 352 33.175 0.010 68.425 1.00 11.62 B ATOM 5125 C TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5126 O TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5127 N ALA 353 36.115 -5.822 66.407 1.00 19.93 B ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 35.406 -5.891 63.951 1.00 16.39 B ATOM 5130 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.224 63.365 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 35.761 -10.712 64.509 1.00 20.34 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.294 1.00 20.34 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5139 NE2 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5139 NE2 HIS 354 34.897 -13.031 65.156 1.00 25.57 B ATOM 5139 NE2 HIS 354 34.897 -13.031 64.294 1.00 25.34 B ATOM 5139 NE2 HIS 354 34.891 -13.948 63.164 1.00 26.03 B ATOM 5131 O ALA 353 33.486 -9.811 64.796 1.00 20.24 B ATOM 5134 CB HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5135 CA HIS 354 34.891 -13.948 63.164 1.00 26.03 B ATOM 5136 CD2 HIS 354 34.891 -13.948 63.164 1.00 20.20 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CA ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5140 C HIS 354 34.891 -13.948 63.164 1.00 20.02 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5140 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5140 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5140 NH1 ARG 355 31.461 -7.943 71.673 1.00 21.76 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.12 B ATOM 5151 C ARG 355 30.040 -8.932 66.453 1.00 21.											
40 ATOM 5120 CE1 TYR 352 34.220 -1.649 67.067 1.00 11.17 B ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CE2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5125 C TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 O TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5127 N ALA 353 36.115 -5.822 66.407 1.00 19.93 B ATOM 5128 CA ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 17.31 B ATOM 5130 C ALA 353 36.359 -5.698 62.821 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.229 63.365 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.229 63.365 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 20.34 B ATOM 5136 CD2 HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5137 ND1 HIS 354 35.302 -12.121 64.294 1.00 25.57 B ATOM 5138 CE1 HIS 354 34.797 -9.661 63.994 1.00 22.75 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 25.57 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 25.57 B ATOM 5130 C HIS 354 34.831 -13.948 63.164 1.00 25.57 B ATOM 5134 CB HIS 354 34.831 -13.948 63.164 1.00 25.57 B ATOM 5136 CD2 HIS 354 34.831 -13.948 63.164 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5140 C HIS 354 33.886 -9.811 64.796 1.00 20.23 B ATOM 5140 C HIS 354 33.886 -9.811 64.796 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.255 66.891 1.00 20.70 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5145 CG ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 51510 NH2 ARG 355 31.002 -8.942 72.281 1.00 31.26 B ATOM 51549 NH1 ARG 355 31.002 -8.942 72.281 1.00 31.12 B ATOM 5155 O ARG 355 31.004 -8.932 66.453 1.00 23.53 B											
ATOM 5121 CD2 TYR 352 35.570 -2.654 69.282 1.00 10.15 B ATOM 5122 CE2 TYR 352 34.699 -1.584 69.483 1.00 9.37 B ATOM 5123 CZ TYR 352 34.699 -1.584 69.483 1.00 9.37 B ATOM 5123 CZ TYR 352 34.624 -1.078 68.322 1.00 11.62 B ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5125 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5126 O TYR 352 34.217 -5.852 66.407 1.00 19.93 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 36.315 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 17.31 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5136 CD2 HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.599 1.00 25.57 B ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5139 NEZ HIS 354 34.831 -13.948 63.164 1.00 25.34 B ATOM 5139 NEZ HIS 354 34.831 -13.948 63.164 1.00 20.23 B ATOM 5134 CB HIS 354 34.831 -13.948 63.164 1.00 20.23 B ATOM 5134 CB HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5134 CB HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5134 CB HIS 354 34.831 -13.948 63.164 1.00 20.23 B ATOM 5136 CD2 HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5137 ND1 HIS 354 34.831 -13.948 63.164 1.00 20.23 B ATOM 5140 C HIS 354 34.831 -13.948 63.164 1.00 20.23 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 HS.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 HS.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 HS.53 B ATOM 5144 NARG 355 31.869 -9.255 66.891 1.00 20.76 B ATOM 5145 CG ARG 355 31.869 -9.255 66.891 1.00 20.76 B ATOM 5145 CG ARG 355 31.869 -9.8679 73.262 1.00 31.12 B ATOM 5140 CD ARG 355 31.402 -10.266 71.921 1.00 31.17 B ATOM 5145 CG ARG 355 31.402 -10.266 79.32 1.00 31.12 B ATOM 5150 C ARG 355 31.477 -8.513 66.355 1.00 21.80 B	40										
ATOM 5122 CE2 TYR 352 34.699 -1.584 69.433 1.00 9.37 B ATOM 5123 CZ TYR 352 34.024 -1.078 68.322 1.00 11.62 B ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5127 N ALA 353 36.115 -5.852 66.407 1.00 19.93 B ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5130 C ALA 353 36.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 35.761 -10.712 64.509 1.00 20.34 B ATOM 5135 CG HIS 354 35.791 -10.712 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5138 CE1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5139 NE2 HIS 354 34.811 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.811 -13.948 63.164 1.00 26.03 B ATOM 5134 CB HIS 354 34.811 -14.162 64.427 1.00 26.67 B ATOM 5137 ND1 HIS 354 34.811 -13.948 63.164 1.00 26.03 B ATOM 5138 CE1 HIS 354 34.811 -13.948 63.164 1.00 26.03 B ATOM 5134 CB HIS 354 34.811 -13.948 63.164 1.00 26.03 B ATOM 5134 CB HIS 354 33.543 -9.216 64.297 1.00 20.24 B ATOM 5136 CD2 HIS 354 33.505 -9.255 65.995 1.00 20.27 B ATOM 5137 ND1 HIS 354 33.505 -9.255 65.995 1.00 20.20 B ATOM 5140 C HIS 354 33.505 -9.255 65.995 1.00 20.20 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5144 CB ARG 355 32.823 -8.721 69.339 1.00 21.77 B ATOM 5144 CB ARG 355 30.820 -8.942 72.281 1.00 31.17 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5151 C ARG 355 31.177 -8.513 66.355 1.00 23.53 B											
45 ATOM 5124 OH TYR 352 33.175 0.010 68.445 1.00 11.62 B ATOM 5125 C TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5126 O TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5126 O TYR 352 34.217 -5.852 66.407 1.00 19.93 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5131 O ALA 353 33.542 -7.224 63.785 1.00 18.36 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 35.554 -8.319 64.119 1.00 19.39 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5137 ND1 HIS 354 35.302 -12.121 64.294 1.00 25.57 B ATOM 5138 CEI HIS 354 34.779 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.302 -12.121 64.294 1.00 25.57 B ATOM 5138 CEI HIS 354 34.831 -12.725 63.053 1.00 25.77 B ATOM 5137 ND1 HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5138 CEI HIS 354 34.831 -12.725 63.053 1.00 25.77 B ATOM 5140 C HIS 354 33.481 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.481 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.505 -9.255 65.995 1.00 20.23 B ATOM 5140 C HIS 354 33.505 -9.255 65.995 1.00 20.24 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 20.20 B ATOM 5147 ND1 HIS 354 32.512 -10.417 64.352 1.00 20.20 B ATOM 5147 ND1 HIS 354 32.512 -10.417 64.352 1.00 20.20 B ATOM 5147 ND1 HIS 354 32.512 -10.417 64.352 1.00 20.20 B ATOM 5147 ND1 HIS 354 32.512 -10.417 64.352 1.00 20.20 B ATOM 5147 ND1 HIS 354 32.512 -10.417 64.352 1.00 20.20 B ATOM 5148 CZ ARG 355 32.370 -9.285 66.891 1.00 20.20 B ATOM 5148 CZ ARG 355 33.505 -9.255 65.995 1.00 20.70 B ATOM 5148 CZ ARG 355 31.899 -8.677 69.339 1.00 21.77 B ATOM 5148 CZ ARG 355 31.402 -10.206 71.921 1.00 3											
45 ATOM 5125 C TYR 352 33.175 0.010 68.445 1.00 14.22 B ATOM 5125 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5126 O TYR 352 34.217 -5.852 66.407 1.00 19.93 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5135 CG HIS 354 35.361 -10.712 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.362 -12.121 64.294 1.00 25.34 B ATOM 5137 ND1 HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5139 NE2 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5130 C C HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5130 C C HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5146 CD ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 31.461 -7.943 7.10673 1.00 27.66 B ATOM 5147 NE ARG 355 31.461 -7.943 7.16673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.12 B ATOM 5149 NH1 ARG 355 30.820 -8.942 72.281 1.00 31.12 B ATOM 5150 NH2 ARG 355 30.820 -8.942 72.281 1.00 31.12 B ATOM 5150 NH2 ARG 355 30.040 -8.942 72.281 1.00 31.12 B ATOM 5150 NH2 ARG 355 30.040 -8.942 72.281 1.00 31.12 B ATOM 5150 NH2 ARG 355 30.040 -8.942 72.281 1.00 21.553 B											
45 ATOM 5125 C TYR 352 35.442 -5.814 66.362 1.00 18.80 B ATOM 5126 O TYR 352 34.217 -5.852 66.407 1.00 19.93 B ATOM 5127 N ALA 353 36.115 -5.852 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 20.34 B ATOM 5135 CG HIS 354 35.362 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 34.979 -9.661 63.994 1.00 20.34 B ATOM 5136 CD2 HIS 354 34.979 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5138 CEI HIS 354 34.979 -13.031 65.156 1.00 25.57 B ATOM 5138 CEI HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.511 -14.162 64.427 1.00 26.667 B ATOM 5140 C HIS 354 34.511 -14.162 64.427 1.00 26.667 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 355 32.370 -9.255 66.891 1.00 20.24 B ATOM 5140 C HIS 355 32.370 -9.255 66.891 1.00 20.70 B ATOM 5146 CD ARG 355 32.370 -9.255 66.891 1.00 20.76 B ATOM 5147 NE ARG 355 32.370 -9.255 66.891 1.00 20.76 B ATOM 5149 NH1 ARG 355 32.433 -8.121 70.598 1.00 21.77 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 30.820 -8.942 72.281 1.00 31.17 B ATOM 5149 NH1 ARG 355 30.820 -8.942 72.281 1.00 31.17 B ATOM 5150 NH2 ARG 355 30.820 -8.942 72.281 1.00 31.17 B ATOM 5150 NH2 ARG 355 30.820 -8.942 72.281 1.00 31.17 B ATOM 5150 NH2 ARG 355 30.040 -8.932 66.453 1.00 23.53 B											
ATOM 5126 O TYR 352 34.217 -5.852 66.407 1.00 19.93 B ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5135 CG HIS 354 35.302 -12.121 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.37 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.831 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 20.24 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 20.20 B ATOM 5144 CB ARG 355 32.823 -8.721 68.299 1.00 20.70 B ATOM 5145 CG ARG 355 32.823 -8.721 68.299 1.00 20.70 B ATOM 5146 CD ARG 355 32.823 -8.721 68.299 1.00 20.76 B ATOM 5147 NE ARG 355 32.823 -8.721 69.339 1.00 27.76 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.12 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 30.040 -8.932 66.453 1.00 23.53 B	45										
ATOM 5127 N ALA 353 36.115 -5.822 65.216 1.00 18.33 B ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5136 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5130 N2 HIS 354 34.831 -13.948 63.164 1.00 26.67 B ATOM 5140 C HIS 354 34.831 -13.948 63.164 1.00 26.67 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5144 CB ARG 355 32.370 -9.285 66.891 1.00 20.70 B ATOM 5146 CD ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5146 CD ARG 355 31.789 -8.672 69.339 1.00 22.76 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B											
ATOM 5128 CA ALA 353 35.406 -5.891 63.951 1.00 17.31 B ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5135 CG HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5140 C HIS 354 34.831 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5142 N ARG 355 33.505 -9.255 66.891 1.00 20.70 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.70 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5147 NE ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5149 NH1 ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B											
50 ATOM 5129 CB ALA 353 36.359 -5.698 62.821 1.00 16.39 B ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5135 CG HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.811 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5142 N ARG 355 32.370 -9.285 66.891 1.00 20.02 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.70 B ATOM 5146 CD ARG 355 32.370 -9.285 66.891 1.00 20.70 B ATOM 5146 CD ARG 355 32.370 -9.285 66.891 1.00 20.70 B ATOM 5147 NE ARG 355 32.433 -8.121 70.598 1.00 27.76 B ATOM 5148 CZ ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5151 C ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B											
50 ATOM 5130 C ALA 353 34.680 -7.221 63.785 1.00 18.36 B ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.509 1.00 22.75 B ATOM 5136 CD2 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.511 -14.162 64.427											
ATOM 5131 O ALA 353 33.542 -7.249 63.365 1.00 18.10 B ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5135 CG HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 35.302 -12.121 64.294 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.831 -13.948 63.164 1.00 26.67 B ATOM 5140 C HIS 354 34.831 -14.162 64.427 1.00 26.67 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 22.76 B ATOM 5146 CD ARG 355 31.461 -7.943 71.673 1.00 27.666 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B	50										
ATOM 5132 N HIS 354 35.354 -8.319 64.119 1.00 19.39 B ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5135 CG HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.946 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.831 -13.946 63.164 1.00 26.67 B ATOM 5140 C HIS 354 34.831 -14.162 64.427 1.00 26.67 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 32.370 -9.285 66.891 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.766 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.666 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.042 -8.942 72.281 1.00 31.26 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B	50										
ATOM 5133 CA HIS 354 34.779 -9.661 63.994 1.00 20.34 B ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5135 CG HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 34.831 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -12.725 63.053 1.00 25.77 B ATOM 5139 NE2 HIS 354 34.811 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5145 CG ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.766 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.666 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5151 C ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5151 C ARG 355 31.042 -8.513 66.305 1.00 23.53 B											
55 ATOM 5134 CB HIS 354 35.761 -10.712 64.509 1.00 22.75 B ATOM 5135 CG HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5146 CD ARG 355 31.789 -8.672 69.339 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.26 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B											
55 ATOM 5135 CG HIS 354 35.302 -12.121 64.294 1.00 25.34 B ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 31.789 -8.672 69.339 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B											
ATOM 5136 CD2 HIS 354 34.797 -13.031 65.156 1.00 25.57 B ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.831 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 31.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 23.53 B	55										_
ATOM 5137 ND1 HIS 354 35.311 -12.725 63.053 1.00 25.77 B ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 21.77 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5148 CZ ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B	JJ										
ATOM 5138 CE1 HIS 354 34.831 -13.948 63.164 1.00 26.03 B ATOM 5139 NE2 HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B											
60 ATOM 5139 NE2 HIS 354 34.511 -14.162 64.427 1.00 26.67 B ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 23.53 B											-
60 ATOM 5140 C HIS 354 33.486 -9.811 64.796 1.00 20.23 B ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5145 CG ARG 355 32.370 -9.285 66.891 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 20.70 B ATOM 5145 CD ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.766 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.666 B ATOM 5149 NH1 ARG 355 31.461 -7.943 71.673 1.00 27.666 B ATOM 5149 NH1 ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.042 -8.874 72.281 1.00 31.17 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B											
ATOM 5141 O HIS 354 32.512 -10.417 64.352 1.00 18.53 B ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 31.042 -10.206 71.921 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B	60										
ATOM 5142 N ARG 355 33.505 -9.255 65.995 1.00 20.24 B ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B	OU ·										В
ATOM 5143 CA ARG 355 32.370 -9.285 66.891 1.00 20.90 B ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B											В
65 ATOM 5144 CB ARG 355 32.823 -8.721 68.239 1.00 20.70 B ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B											В
65 ATOM 5145 CG ARG 355 31.789 -8.672 69.339 1.00 21.77 B ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 <											
ATOM 5146 CD ARG 355 32.433 -8.121 70.598 1.00 22.76 B ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B	45										
ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B	O)										В
70 ATOM 5147 NE ARG 355 31.461 -7.943 71.673 1.00 27.66 B ATOM 5148 CZ ARG 355 30.820 -8.942 72.281 1.00 31.26 B ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B				CD			32.433	-8.121	70.598		В
70 ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B										1.00 27.66	В
70 ATOM 5149 NH1 ARG 355 31.042 -10.206 71.921 1.00 31.17 B ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B							30.820	-8.942		1.00 31.26	B
70 ATOM 5150 NH2 ARG 355 29.965 -8.679 73.262 1.00 31.12 B ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B	7 0			NH1	ARG	355	31.042	-10.206	71.921	1.00 31.17	
ATOM 5151 C ARG 355 31.177 -8.513 66.305 1.00 21.80 B ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B	/0			NH2	ARG					1.00 31.12	
ATOM 5152 O ARG 355 30.040 -8.932 66.453 1.00 23.53 B			5151	С	ARG	355	31.177		66.305		
				Ο,	ARG		30.040	-8.932	66.453		
		MOTA	5153	N	ALA	356 ·	31.442	-7.394	65.634	1.00 21.31	В

ATOM 5155 C ALA 356 30.936 -5.826 65.099 1.00 20.58 ATOM 5155 C ALA 356 30.936 -7.256 63.902 1.00 20.58 ATOM 5155 C ALA 356 356 30.936 -7.256 63.902 1.00 20.58 ATOM 5158 C ALA 356 356 30.936 -7.256 63.902 1.00 20.58 ATOM 5158 C ALA 356 72 80.935 -6.328 63.902 1.00 20.58 ATOM 5158 C ALA 356 72 80.935 -6.328 63.902 1.00 20.58 ATOM 5158 C ALYS 357 20.935 -9.981 62.245 1.00 22.88 ATOM 5160 CB LYS 357 30.347 -10.371 61.191 1.00 23.14 ATOM 5160 CB LYS 357 30.347 -10.371 61.191 1.00 23.14 ATOM 5161 CG LYS 357 30.347 -10.371 61.191 1.00 23.14 ATOM 5162 CD LYS 357 31.897 -10.597 59.981 1.00 27.85 ATOM 5162 CD LYS 357 31.897 -10.597 59.981 1.00 27.85 ATOM 5164 NZ LYS 357 32.648 -12.966 60.485 1.00 27.32 ATOM 5166 C LYS 357 28.8198 -9.551 62.594 1.00 23.74 ATOM 5165 C LYS 357 28.8198 -9.551 62.594 1.00 23.74 ATOM 5166 C LYS 357 28.8198 -9.551 62.594 1.00 23.74 ATOM 5166 C LYS 357 27.315 -9.635 61.755 1.00 22.43 ATOM 5166 C LYS 357 27.315 -9.635 61.755 1.00 22.43 ATOM 5166 C ANN 358 26.730 -10.306 64.388 1.00 22.82 ATOM 5160 CB ANN 358 26.530 -10.306 64.388 1.00 22.58 ATOM 5170 CG ANN 358 26.530 -11.00 66 43.88 1.00 22.99 74 ATOM 5170 CG ANN 358 27.852 -12.105 65.766 1.00 28.23 ATOM 5170 CG ANN 358 27.852 -12.105 65.766 1.00 28.23 ATOM 5170 CG ANN 358 28.2607 -3.279 64.476 1.00 30.99 74 ATOM 5177 CG ANN 358 28.2607 -3.279 64.476 1.00 30.99 74 ATOM 5177 CG ANN 358 28.2607 -3.279 64.476 1.00 30.99 74 ATOM 5177 CG ANN 358 28.2607 -3.279 64.476 1.00 30.99 74 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.2607 -3.279 64.476 1.00 30.39 ATOM 5177 CG ANN 358 29.220 2.00 30.90 ATOM 5177 CG ANN 358 29.220 2.00 30.90 ATOM 5177 CG AN						256	20 275	5 505	c= 040		_
5 ATOM 5155 C ALA 3556 28.531 -6.796 63.902 1.00 20.99 ATOM 5157 0 ALA 3556 28.531 -6.796 63.543 1.00 19.69 ATOM 5159 C ALVS 357 30.195 -8.328 63.340 1.00 22.58 ATOM 5159 C ALVS 357 30.195 -8.328 63.340 1.00 22.58 ATOM 5161 CC LVS 357 30.347 -10.371 61.911 1.00 23.14 ATOM 5161 CC LVS 357 31.677 -10.194 61.443 1.00 25.46 ATOM 5163 CC LVS 357 31.677 -10.194 61.443 1.00 25.46 ATOM 5163 CC LVS 357 31.687 -10.1959 59.993 1.00 27.26 ATOM 5163 CC LVS 357 31.680 -12.104 59.5763 1.00 27.26 ATOM 5165 C LVS 357 31.680 -12.104 59.5763 1.00 27.26 ATOM 5165 C LVS 357 31.680 -12.104 59.563 1.00 27.26 ATOM 5165 C LVS 357 32.648 -12.966 60.485 1.00 27.32 ATOM 5166 0 LVS 357 28.198 9.551 62.594 1.00 23.74 ATOM 5165 C LVS 357 28.198 9.551 62.594 1.00 23.74 ATOM 5167 N ASN 358 22.016 -9.885 63.866 1.00 25.58 ATOM 5167 N ASN 358 22.016 -9.885 63.866 1.00 25.58 ATOM 5167 N ASN 358 22.016 -9.885 63.866 1.00 25.58 ATOM 5170 CO SN 358 22.02 1.00 20.00 20.97 ATOM 5171 OOL ASN 358 28.25 21.210 56.64 28.29 ATOM 5171 OOL ASN 358 28.25 21.2105 66.742 1.00 29.97 ATOM 5172 C ASN 358 28.25 21.2105 66.5742 1.00 29.97 ATOM 5172 C ASN 358 28.25 20.00 29.270 64.476 1.00 30.00 ATOM 5177 C B LUE 359 22.695 -0.906 64.551 1.00 30.00 ATOM 5177 C B LUE 359 24.655 -6.966 64.166 1.00 30.09 ATOM 5178 C G2 LUE 359 24.655 -6.966 64.176 1.00 30.09 ATOM 5180 CD LUE 359 22.6375 -5.433 65.361 1.00 32.19 ATOM 5180 CD LUE 359 24.655 -6.966 64.176 1.00 30.19 ATOM 5180 CD LUE 359 24.655 -6.966 64.176 1.00 30.19 ATOM 5180 CD LUE 359 24.655 -6.966 64.176 1.00 30.19 ATOM 5180 CD LUE 359 24.655 -6.966 64.176 1.00 30.19 ATOM 5180 CD LUE 359 24.656 -7.255 60.00 64.176 1.00 31.11 ATOM 5180 CD LUE 359 24.656 -7.255 60.00 64.176 1.00 31.11 ATOM 5180 CD LUE 359 24.656 -7.256 64.365 1.00 31.11 ATOM 5180 CD LUE 359 24.656 -7.966 64.176 1.00 31.91 ATOM 5180 CD LUE 359 24.656 -7.956 64.365 1.00 31.91 ATOM 5180 CD LUE 359 24.656 -7.956 64.365 1.00 31.91 ATOM 5180 CD LUE 359 24.656 -7.956 64.365 1.00 31.91 ATOM 5180 CD LUE 359 24.656 -7.956 64.365 1.00 31.91 ATOM 5180 CD LUE 359 24		MOTA	5154	CA	ALA	356	30.375	-6.586	65.049	1.00 20.41	В
ATOM 5159 CA LVS 357 30.195 -8.328 63.340 1.00 19.69 ATOM 5159 CA LVS 357 30.195 -8.328 63.340 1.00 22.58 ATOM 5150 CE LVS 357 30.347 -10.371 61.911 1.00 23.14 ATOM 5162 CD LVS 357 31.877 -10.579 59.983 1.00 23.14 ATOM 5162 CD LVS 357 31.877 -10.579 59.983 1.00 27.85 ATOM 5164 CA LVS 357 31.877 -10.579 59.983 1.00 27.85 ATOM 5164 CA LVS 357 31.866 -12.104 59.763 1.00 27.26 ATOM 5164 CA LVS 357 32.648 -12.966 60.485 1.00 27.32 ATOM 5164 CA LVS 357 32.648 -12.966 60.485 1.00 27.32 ATOM 5166 CA LVS 357 32.648 -12.966 60.485 1.00 27.32 ATOM 5166 CA LVS 357 27.315 -9.635 61.755 1.00 22.43 ATOM 5166 CA LVS 357 27.315 -9.635 61.755 1.00 22.43 ATOM 5168 CA ASN 358 26.730 -10.397 64.388 1.00 28.23 ATOM 5168 CA ASN 358 26.730 -10.396 64.388 1.00 28.23 ATOM 5168 CA ASN 358 26.914 -10.928 65.766 1.00 28.39 ATOM 5170 CD ASN 358 27.852 -12.105 65.742 1.00 29.97 ATOM 5171 CO ASN 358 22.212.105 65.742 1.00 29.97 ATOM 5171 CO ASN 358 22.4487 -9.619 64.466 1.00 30.93 ATOM 5172 CD ASN 358 22.4487 -9.619 64.666 1.00 30.93 ATOM 5172 CD ASN 358 22.4487 -9.619 64.666 1.00 30.93 ATOM 5175 CD ASN 358 22.4487 -9.619 64.666 1.00 30.93 ATOM 5177 CD ASN 358 22.4487 -9.619 64.666 1.00 30.93 ATOM 5178 CD LLE 359 25.892 -8.011 6.152 1.00 31.15 ATOM 5177 CD LLE 359 25.892 -8.011 6.152 1.00 31.15 ATOM 5178 CD LLE 359 25.4855 -5.696 64.176 1.00 31.93 ATOM 5178 CD LLE 359 25.4855 -5.604 64.162 1.00 31.93 ATOM 5181 CD LLE 359 22.4855 -5.604 64.162 1.00 31.93 ATOM 5181 CD LLE 359 22.4855 -5.604 64.162 1.00 31.93 ATOM 5181 CD LLE 359 22.4855 -5.604 64.162 1.00 31.93 ATOM 5181 CD LLE 359 22.4855 -5.604 64.162 1.00 31.93 ATOM 5180 CD LLE 359 22.4855 -5.604 64.162 1.00 31.93 ATOM 5180 CD LLE 359 22.4855 -5.604 64.162 1.00 31.93 ATOM 5180 CD LLE 359 22.4366 -7.355 64.134 1.00 31.93 ATOM 5180 CD LLE 359 22.4366 -7.355 64.134 1.00 31.93 ATOM 5180 CD LLE 359 22.10 360 22.606 0.735 64.104 1.00 31.93 ATOM 5180 CD LLE 360 20.00 36.275 55.50 56.10 1.00 31.93 ATOM 5180 CD LLE 360 20.00 36.275 55.50 56.10 1.00 31.93 ATOM 5180 CD LLE 360 20.00 36.275 55.50 56.10											В .
5 ATOM 5159 N. LYS 357 30.195 -8.328 63.340 1.00 22.58 ATOM 5159 CA. LYS 357 29.550 -9.081 62.225 1.00 22.82 ATOM 5161 CG LYS 357 30.347 -10.371 61.911 1.00 23.14 ATOM 5161 CG LYS 357 31.67 -10.194 61.443 1.00 25.46 1.00 25.46 1.00 25.45 1.00											B
ATOM 5160 CB LVS 357 30.347 -10.371 61.911 1.00 23.14 ATOM 5162 CB LVS 357 30.347 -10.371 61.911 1.00 23.14 ATOM 5162 CB LVS 357 31.867 -10.194 61.443 1.00 23.46 ATOM 5163 CE LVS 357 31.867 -10.194 61.443 1.00 27.85 ATOM 5164 NZ LVS 357 31.660 -12.104 59.763 1.00 27.85 ATOM 5165 CB LVS 357 32.648 -12.966 60.485 1.00 27.32 ATOM 5166 NZ LVS 357 32.648 -12.966 60.485 1.00 27.32 ATOM 5166 NZ LVS 357 22.315 -9.635 62.594 1.00 27.32 ATOM 5166 NZ LVS 357 22.315 -9.635 62.594 1.00 27.32 ATOM 5166 NZ LVS 357 27.315 -9.635 62.594 1.00 27.32 ATOM 5168 CA ASN 358 26.730 -10.306 63.98 1.00 28.23 ATOM 5169 CB ASN 358 26.730 -10.306 63.98 1.00 28.23 ATOM 5170 CG ASN 358 26.914 -10.928 65.766 1.00 28.39 ATOM 5171 ODI ASN 358 28.203 -12.649 66.778 1.00 31.69 ATOM 5172 NZ ASN 358 28.203 -12.649 66.778 1.00 31.69 ATOM 5173 C ASN 358 28.256 60 -9.270 64.476 1.00 30.00 ATOM 5174 O ASN 358 22.637 -12.506 64.551 1.00 30.00 ATOM 5177 CB ILE 359 25.892 -8.011 66.152 1.00 31.11 ATOM 5178 CG2 ILE 359 24.655 -6.986 61.766 1.00 32.09 ATOM 5179 CG1 ILE 359 24.655 -6.986 61.766 1.00 32.09 ATOM 5179 CG1 ILE 359 24.657 -4.569 61.366 1.00 31.91 ATOM 5180 CD1 ILE 359 22.6375 -5.433 65.361 1.00 32.12 ATOM 5180 CD1 ILE 359 22.6375 -5.433 65.361 1.00 32.12 ATOM 5180 CD ILE 359 24.357 -4.559 61.366 1.00 34.29 ATOM 5180 CD ILE 359 24.356 -6.986 61.366 1.00 34.29 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.12 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.03 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 32.03 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 33.89 ATOM 5180 CD ILE 359 24.367 -4.559 61.361 1.00 33.89 ATOM 5180 CD	5										В
ATOM 5160 CB LYS 357 30.347 -10.371 61.911 1.00 23.14 ATOM 5161 CC LYS 357 31.897 -10.194 61.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 25.46 1.443 1.00 27.26	,										В
ATOM \$162 CD LYS \$357 \$31.767 10.194 \$61.443 1.00 25.46 ATOM \$162 CD LYS \$357 \$31.867 10.597 \$59.989 1.00 27.25 ATOM \$164 CD LYS \$357 \$31.660 -12.104 \$59.763 1.00 27.25 ATOM \$165 CD LYS \$357 \$28.198 -9.551 \$62.594 1.00 23.74 ATOM \$166 CD LYS \$357 \$28.198 -9.551 \$62.594 1.00 23.74 ATOM \$166 CD LYS \$357 \$28.198 -9.551 \$62.594 1.00 23.74 ATOM \$166 CD LYS \$357 \$28.198 -9.551 \$61.755 1.00 22.43 ATOM \$166 CD LYS \$357 \$28.198 -9.551 \$61.795 1.00 22.43 ATOM \$167 N ASN \$358 \$28.016 -9.845 \$61.795 1.00 22.43 ATOM \$3169 CB ASN \$358 \$26.914 -10.928 \$65.766 1.00 28.39 ATOM \$3170 CD ASN \$358 \$26.914 -10.928 \$65.766 1.00 28.39 ATOM \$3171 CD ASN \$358 \$28.203 -12.649 \$64.785 1.00 29.97 ATOM \$3172 CD ASN \$358 \$28.203 -12.649 \$64.785 1.00 29.57 ATOM \$3175 CD ASN \$358 \$25.606 -9.270 \$64.476 1.00 30.00 ATOM \$3175 CD ASN \$358 \$25.606 -9.270 \$64.476 1.00 30.00 ATOM \$3175 CD ASN \$358 \$25.606 -9.270 \$64.476 1.00 30.00 ATOM \$3177 CD ASN \$358 \$25.606 -9.270 \$64.476 1.00 30.93 ATOM \$3177 CD ASN \$359 \$24.655 -5.604 \$64.152 1.00 31.11 ATOM \$3177 CD ASN \$359 \$24.655 -5.604 \$64.142 1.00 31.31 ATOM \$3177 CD ASN \$359 \$24.655 -5.604 \$64.142 1.00 31.91 ATOM \$3179 CD ASN \$359 \$24.655 -5.604 \$64.142 1.00 31.91 ATOM \$3179 CD ASN \$359 \$24.655 -5.604 \$64.142 1.00 31.91 ATOM \$3179 CD ASN \$360 \$25.655 -5.604 \$64.142 1.00 31.91 ATOM \$3180 CD ASN \$360 \$25.655 -5.604 \$64.142 1.00 31.91 ATOM \$3180 CD ASN \$360 \$25.655 -5.604 \$64.142 1.00 31.91 ATOM \$3180 CD ASN \$360 \$26.655 -5.604 \$64.142 1.00 31.91 ATOM \$3180 CD ASN \$360 \$26.655 -5.604 \$64.142 1.00 31.91 ATOM \$3180 CD ASN \$360 \$25.655 -5.604 \$64.142 1.00 31.91 ATOM											В
10 ATOM \$163 CC LYS 357 31.897 -10.597 59.983 1.00 27.85 ATOM \$163 CC LYS 357 32.668 -12.966 60.485 1.00 27.32 ATOM \$165 C LYS 357 32.668 -12.966 60.485 1.00 27.32 ATOM \$165 C LYS 357 28.198 -9.551 62.594 1.00 22.74 ATOM \$166 C LYS 357 28.198 -9.551 62.594 1.00 22.74 ATOM \$166 C LYS 357 28.198 -9.551 62.594 1.00 22.74 ATOM \$166 C LYS 357 27.315 -9.635 61.755 1.00 22.43 ATOM \$166 C LYS 357 27.315 -9.635 61.755 1.00 22.43 ATOM \$167 C A SNN 358 28.016 -9.865 63.876 1.00 22.55 ATOM \$167 C B ASN 358 26.730 -10.306 64.388 1.00 22.43 ATOM \$1570 CG ASN 358 26.730 -10.306 64.388 1.00 22.33 ATOM \$1570 CG ASN 358 27.852 -12.105 65.742 1.00 29.97 ATOM \$1571 CG ASN 358 28.267 -12.506 64.551 1.00 29.57 ATOM \$1571 C ASN 358 28.267 -12.506 64.551 1.00 29.57 ATOM \$1572 NDZ ASN 358 28.267 -12.506 64.551 1.00 30.93 ATOM \$1574 C ASN 358 28.267 -12.506 64.551 1.00 30.93 ATOM \$1576 CA ILLE 359 24.855 -6.986 64.176 1.00 30.93 ATOM \$1576 CA ILLE 359 24.855 -6.986 64.176 1.00 30.93 ATOM \$1576 CA ILLE 359 24.855 -6.986 64.176 1.00 32.09 ATOM \$1576 CA ILLE 359 24.367 -4.569 64.136 1.00 30.39 ATOM \$1576 CA ILLE 359 24.367 -4.569 64.136 1.00 30.39 ATOM \$1570 CG ILLE 359 27.169 -4.334 65.361 1.00 32.12 ATOM \$1580 CDI ILLE 359 27.169 -4.334 65.361 1.00 32.12 ATOM \$1580 CDI ILLE 359 27.169 -4.334 65.361 1.00 32.83 ATOM \$1580 CDI ILLE 359 27.169 -4.334 65.361 1.00 32.83 ATOM \$1580 CDI ILLE 359 24.366 -7.355 61.843 1.00 32.83 ATOM \$1580 CDI ILLE 359 24.366 -7.355 61.843 1.00 32.83 ATOM \$1580 CDI ILLE 360 20.60 ATOM \$1590 CDI ASN 361 20.80 ATOM \$1590											В
10 ATOM 5166 CE LYS 357 ATOM 5166 NZ LYS 357 ATOM 5167 N ASN 358 28.016 -9.845 63.876 1.00 22.14 ATOM 5168 NZ ASN 358 ATOM 5169 NZ ASN 358 ATOM 5169 NZ ASN 358 ATOM 5170 NZ ASN 358 ATOM 5170 NZ ASN 358 ATOM 5171 NZ ASN 358 ATOM 5172 NZ ASN 358 ATOM 5173 NZ ASN 358 ATOM 5175 NZ LZ											В
ATOM 5166 NZ LYS 357	10										В
ATOM \$166 C LYS 357 28.198 -9.551 62.594 1.00 22.43	10										В
ATOM 5166 O LYS 357											· B
ATOM 5167 N ASN 358 28.016 -9.845 63.876 1.00 25.58											В
ATOM \$168 CA ASN 358 26.730 -10.306 64.388 1.00 28.23											В
ATOM \$169 CB ASN 358 26,914 -10,928 65,766 1,00 28,39	15										В
ATOM 5170 CG ASN 358 27.852 - 12.105 65.742 1.00 29.97	13										В
20 ATOM 5171 OD1 ASN 358 28.203 -12.649 66.778 1.00 31.69 ATOM 5173 C ASN 358 25.606 -9.270 64.476 1.00 30.00 ATOM 5173 C ASN 358 25.606 -9.270 64.476 1.00 30.00 ATOM 5175 N ILE 359 25.892 -8.011 64.152 1.00 31.11 ATOM 5176 CA ILE 359 24.855 -6.986 64.176 1.00 32.09 ATOM 5177 CB ILE 359 24.855 -6.986 64.176 1.00 32.09 ATOM 5177 CB ILE 359 24.855 -6.986 64.176 1.00 32.09 ATOM 5178 CG2 ILE 359 24.367 -4.569 64.136 1.00 32.09 ATOM 5178 CG2 ILE 359 24.367 -4.569 64.136 1.00 32.12 ATOM 5179 CG1 ILE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5180 CD1 ILE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5180 CD1 ILE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5181 C ILE 359 23.393 -7.152 62.984 1.00 33.89 ATOM 5181 C ILE 359 23.093 -7.152 62.984 1.00 33.89 ATOM 5182 O ILE 359 24.326 -7.355 61.843 1.00 32.83 ATOM 5182 C ILE 360 22.605 -7.000 63.256 1.00 36.27 ATOM 5185 CB LEU 360 20.630 -8.381 62.583 1.00 32.23 ATOM 5186 CG LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5188 CC LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5189 C LEU 360 20.037 -9.122 60.240 1.00 44.94 ATOM 5189 C LEU 360 20.037 -9.122 60.240 1.00 44.94 ATOM 5189 C LEU 360 20.037 -9.122 60.240 1.00 44.70 ATOM 5190 O LEU 360 20.037 -9.122 60.240 1.00 44.70 ATOM 5190 C LEU 360 20.000 -5.970 62.028 1.00 39.70 ATOM 5191 N ASN 361 20.740 -5.509 60.777 1.00 40.33 ATOM 5191 N ASN 361 20.740 -5.509 60.777 1.00 40.33 ATOM 5192 CA ASN 361 20.266 5.249 62.994 1.00 39.55 ATOM 5193 C ASN 361 20.265 -3.358 59.573 1.00 40.62 ATOM 5199 C ASN 361 22.993 -2.087 59.792 1.00 41.21 ATOM 5199 C ASN 361 22.993 -2.087 59.792 1.00 41.21 ATOM 5199 N LSS 362 16.572 -3.687 58.975 1.00 41.33 ATOM 5199 C ASN 361 22.993 -2.087 59.792 1.00 41.33 ATOM 5199 C ASN 361 22.199 -3.199 60.777 1.00 40.33 ATOM 5199 C ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5199 N LSS 362 16.572 -3.687 58.975 1.00 40.90 ATOM 5200 CA LVS 362 16.572 -3.687 58.975 1.00 40.90 ATOM 5200 CA LVS 362 16.572 -3.687 58.975 1.00 40.90 ATOM 5200 CA LVS 362 16.592 -3.388 59.573 1.00 40.60 ATOM 5200 CA LVS 362 15.540 4.988 59.595 1.00											В
20 ATOM 5172 ND2 ASN 358 28.267 -12.506 64.551 1.00 29.57 ATOM 5173 C ASN 358 25.606 -9.270 64.476 1.00 30.00 ATOM 5174 O ASN 358 24.487 -9.619 64.845 1.00 30.00 ATOM 5175 N ILE 359 25.892 -8.011 64.152 1.00 31.11 ATOM 5176 CA ILE 359 24.855 -6.6986 64.176 1.00 32.09 ATOM 5177 CB ILE 359 25.4855 -5.604 64.142 1.00 31.91 ATOM 5178 CG2 ILE 359 24.865 -5.604 64.142 1.00 31.91 ATOM 5179 CG1 ILE 359 26.375 -5.433 65.361 1.00 32.09 ATOM 5180 CD1 ILE 359 27.169 -41.134 65.382 1.00 34.29 ATOM 5180 C ILE 359 23.903 -7.152 62.984 1.00 33.89 ATOM 5181 C ILE 359 23.903 -7.152 62.984 1.00 33.89 ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5185 CB LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5186 CG LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CG LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CG LEU 360 20.073 -9.122 60.240 1.00 44.94 ATOM 5189 CD LEU 360 20.073 -9.122 60.240 1.00 44.94 ATOM 5189 CD LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5189 CD LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5189 CD LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5189 CD LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5191 CB ASN 361 20.710 -5.509 60.777 1.04 03.33 ATOM 5190 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5191 CB ASN 361 20.710 -5.509 60.777 1.04 03.33 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 CB LEU 360 20.800 ATOM 5190 CB LEU 360 20.800 ATO											В
ATOM 5173 C ASN 358 25.606 -9.270 64.476 1.00 30.00 AND ATOM 5175 N LLE 359 24.487 -9.619 64.485 1.00 30.93 ATOM 5175 N LLE 359 24.887 -9.619 64.485 1.00 30.93 ATOM 5176 CA LLE 359 24.855 -6.886 64.176 1.00 31.11 ATOM 5176 CA LLE 359 24.855 -6.886 64.176 1.00 31.21 ATOM 5177 CB LLE 359 24.855 -5.604 64.122 1.00 31.91 ATOM 5178 CG2 LLE 359 24.855 -5.604 64.122 1.00 31.91 ATOM 5170 CG1 LLE 359 25.455 -5.604 64.126 1.00 32.12 ATOM 5180 CD1 LLE 359 26.375 -5.433 65.361 1.00 32.12 ATOM 5180 CD1 LLE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5181 C LLE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5181 C LLE 359 27.169 -7.152 66.984 1.00 33.89 ATOM 5182 O LLE 359 24.326 -7.355 61.843 1.00 32.83 ATOM 5183 N LEU 360 22.605 -7.050 63.256 1.00 36.27 ATOM 5184 CA LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5188 CD2 LEU 360 20.073 -9.122 60.240 1.00 44.94 ATOM 5188 CD2 LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5189 C LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.55 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5192 CA ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5193 CB ASN 361 20.710 -5.509 60.777 1.00 40.39 ATOM 5193 CB ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5195 CD ASN 361 18.660 -5.429 62.994 1.00 39.55 ATOM 5195 CD ASN 361 18.660 -5.429 62.994 1.00 39.55 ATOM 5195 CD ASN 361 18.660 -5.429 62.994 1.00 39.55 ATOM 5195 CD ASN 361 18.660 -5.429 62.994 1.00 39.55 ATOM 5195 CD ASN 361 18.660 -5.429 62.994 1.00 39.55 ATOM 5195 CD ASN 361 18.660 -5.429 62.994 1.00 39.55 ATOM 5195 CD ASN 361 18.748 -4.575 59.575 1.00 40.40 40.40 ATOM 5195 CD ASN 361 18.660 -5.429 62.994 1.00 39.55 ATOM 5200 CD ASN 361 18.660 -5.676 6.505 CO ATOM 5200 CD ASN 361 18.660 -5.676 6.585 CO ATOM 5200 CD ASN 361 18.660 -5.676 6.585 CO ATOM 5200 CD ASN 361 18.660 -5.675 6.585 CO ATOM 5200 CD ASN 362 17.283 -2.285 59.575 1.00 40.40 40.40 ATOM 5200 CD ASN 362 17.283 -2.285 59.575 1.00 40.30 ATO											В
ATOM 5174 O ASN 358 24.487 -9.619 64.845 1.00 30.93 ATOM 5175 N LLE 359 25.892 -8.011 64.152 1.00 31.11 ATOM 5176 CA ILE 359 24.855 -6.986 64.176 1.00 32.09 ATOM 5177 CB ILE 359 24.855 -6.986 64.176 1.00 32.09 ATOM 5178 CG2 ILE 359 24.367 -4.559 64.136 1.00 30.39 ATOM 5179 CG1 ILE 359 26.375 -5.433 65.361 1.00 30.39 ATOM 5180 CD1 ILE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5181 C ILE 359 23.903 -7.152 62.984 1.00 33.89 ATOM 5181 C ILE 359 23.903 -7.152 62.984 1.00 33.89 ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 34.29 ATOM 5184 CA LEU 360 22.605 -7.080 63.256 1.00 32.23 ATOM 5185 CB LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CD LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CD LEU 360 20.630 -8.381 62.583 1.00 44.70 ATOM 5188 CD LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5189 C LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5190 C LEU 360 20.280 -5.970 62.281 1.00 39.70 ATOM 5191 N ASN 361 20.780 -5.970 62.028 1.00 39.70 ATOM 5191 N ASN 361 20.780 -5.970 60.777 1.00 40.33 ATOM 5192 CA ASN 361 20.800 -5.970 60.777 1.00 40.33 ATOM 5193 CB ASN 361 22.050 -2.788 60.350 1.00 41.69 ATOM 5194 CG ASN 361 22.050 -2.788 60.350 1.00 41.69 ATOM 5199 N LYS 362 17.838 -3.604 59.557 1.00 40.10 ATOM 5199 N LYS 362 17.838 -3.604 59.557 1.00 41.33 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 41.78 ATOM 5201 CB LYS 362 17.838 -3.604 59.535 1.00 41.33 ATOM 5202 CG LYS 362 17.838 -3.604 59.535 1.00 40.41.78 ATOM 5203 CD LYS 362 17.838 -3.604 59.535 1.00 40.10 41.78 ATOM 5204 CE LYS 362 17.838 -3.604 59.535 1.00 40.41.78 ATOM 5208 OXT LYS 362 17.838 -3.604 59.535 1.00 41.01 1.33 ATOM 5204 CB LYS 362 17.838 -3.604 59.535 1.00 40.60 ATOM 5204 CB LYS 362 15.544 -4.838 59.277 1.00 41.31 ATOM 5204 CB LYS 362 17.838 -3.604 59.535 1.00 40.60 ATOM 5205 CA LYS 362 15.645 -3.358 59.577 1.00 41.01 1.33 ATOM 5204 CB LYS 362 17.838 -3.604 59.535 1.00 40.60 40.70 ATOM 5205 CB LYS 362 15.646 -4.833 59.222 1.00 40.02 40.70 ATOM 5206 CC LYS 362 17.836 -5.875 59.575 1.00 24.130 ATOM 5207 CB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM	20										В
ATOM 5175 N LLE 359 25.892 -8.011 64.152 1.00 31.11 ATOM 5176 CA LLE 359 24.855 -6.986 64.176 1.00 32.09 ATOM 5178 CG2 LLE 359 24.855 -5.604 64.176 1.00 32.09 ATOM 5178 CG2 LLE 359 25.465 -5.604 64.121 1.00 31.91 ATOM 5180 CG2 LLE 359 26.375 -5.433 65.361 1.00 32.12 ATOM 5180 CD1 LLE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5181 C LLE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5183 N LEU 360 22.605 -7.050 62.984 1.00 33.89 ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5184 CA LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5185 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CD LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5187 CD1 LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CD LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CD LEU 360 20.073 -9.122 60.240 1.00 44.94 ATOM 5186 CD LEU 360 20.073 -9.122 60.240 1.00 44.94 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.55 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.55 ATOM 5191 N ASN 361 20.286 -5.429 62.994 1.00 39.55 ATOM 5192 CA ASN 361 20.856 -4.29 62.994 1.00 39.55 ATOM 5193 CB ASN 361 20.856 -3.388 59.573 1.00 40.62 ATOM 5194 CG ASN 361 22.855 -7.298 60.350 1.00 41.21 ATOM 5196 ND2 ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5197 C ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5198 O ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5199 N ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5199 N ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5198 O ASN 361 18.640 -5.5637 58.974 1.00 41.33 ATOM 5199 N ASN 361 18.640 -5.637 58.974 1.00 41.35 ATOM 5199 N ASN 361 22.893 -2.087 59.792 1.00 40.62 ATOM 5203 CD LYS 362 17.388 -3.604 59.535 1.00 40.40 ATOM 5205 NZ LYS 362 17.388 -3.604 59.535 1.00 40.00 ATOM 5207 CD LYS 362 17.388 -3.604 59.535 1.00 40.00 ATOM 5208 NZ LYS 362 15.544 -4.888 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.544 -4.888 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.544 -4.888 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.540 -7.285 55.557 1.00 24.13 ATOM 5240 O28 ADP 2600 44.998 7.100 60	20										В
ATOM 5176 CA ILE 359											В
25 ATOM 5170 CB ILE 359 25.465 -5.604 64.142 1.00 31.91 ATOM 5170 CG2 ILE 359 24.367 -4.569 64.336 1.00 30.39 ATOM 5180 CD1 ILE 359 26.375 -5.433 65.361 1.00 32.12 ATOM 5180 CD1 ILE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5180 CD1 ILE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5182 0 ILE 359 22.903 7.152 62.984 1.00 33.89 ATOM 5182 0 ILE 359 24.326 -7.355 61.843 1.00 32.83 ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5185 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5187 CB LEU 360 20.073 -9.122 60.240 1.00 44.94 ATOM 5187 CD1 LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 0 LEU 360 20.800 -5.970 62.028 1.00 39.75 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5192 CA ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5195 CD ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5197 C ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5197 C ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5198 O ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5198 C ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5197 C ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5197 C ASN 361 18.630 -5.637 58.974 1.00 41.21 ATOM 5198 O ASN 361 12.893 -2.087 59.792 1.00 41.21 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.21 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 40.40 40 ATOM 5203 CD LYS 362 17.283 -2.687 58.795 1.00 40.04 40 ATOM 5203 CD LYS 362 17.283 -2.687 58.975 1.00 40.39 ATOM 5201 CB LYS 362 17.283 -2.687 58.975 1.00 40.05 40 ATOM 5203 CD LYS 362 17.283 -2.687 58.975 1.00 40.00 40.40 ATOM 5203 CD LYS 362 17.283 -2.687 59.575 1.00 40.39 ATOM 5204 CB LYS 362 17.283 -2.687 59.575 1.00 40.39 ATOM 5205 CD LYS 362 17.283 -2.687 59.575 1.00 40.39 ATOM 5205 CD LYS 362 17.283 -2.687 59.575 1.00 40.90 40.40 ATOM 5205 CD LYS 362 15.544 -4.848 60.404 1.00 33.69 ATOM 5205 CD LYS 362 15.544 -4.848 60.404 1.00 33.69 ATOM 5205 CD LYS 362											В
ATOM 5178 CG2 LE 359 24,367 -4,569 64,136 1,00 30,39 ATOM 5179 CG1 LLE 359 26,375 -5,433 65,361 1,00 32,12 ATOM 5180 CD1 LLE 359 27,169 -4,134 65,382 1,00 34,29 ATOM 5181 C LLE 359 23,903 -7,152 62,984 1,00 32,83 30 ATOM 5183 N LEU 360 22,605 -7,080 63,256 1,00 36,27 ATOM 5184 CA LEU 360 22,605 -7,080 63,256 1,00 39,23 ATOM 5186 CB LEU 360 20,630 -8,381 62,583 1,00 42,29 ATOM 5186 CG LEU 360 20,630 -8,381 62,583 1,00 42,29 ATOM 5187 CD1 LEU 360 20,073 -9,122 60,240 1,00 44,94 ATOM 5189 C LEU 360 20,073 -9,122 60,240 1,00 44,70 ATOM 5189 C LEU 360 20,073 -9,122 60,240 1,00 44,70 ATOM 5190 O LEU 360 20,080 -5,970 62,028 1,00 42,24 ATOM 5190 O LEU 360 20,080 -5,970 62,028 1,00 39,70 ATOM 5190 O LEU 360 20,286 -5,429 62,094 1,00 39,55 ATOM 5191 N ASN 361 20,710 -5,509 60,777 1,00 40,33 ATOM 5193 CB ASN 361 20,710 -5,509 60,777 1,00 40,33 ATOM 5195 OD1 ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5195 OD1 ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -2,798 60,350 1,00 41,69 ATOM 5197 C ASN 361 22,050 -3,578 59,575 1,00 40,62 ATOM 5198 D ASN 361 22,050 -3,578 59,575 1,00 40,62 ATOM 5200 C LYS 362 15,544 -1,182 54,828 1,00 31,66 ATOM 5											В
ATOM 5179 C01 ILE 359 26.375 -5.433 65.361 1.00 32.12 ATOM 5180 CD1 ILE 359 27.169 -4.134 65.382 1.00 34.29 ATOM 5181 C ILE 359 23.903 -7.152 62.984 1.00 34.29 ATOM 5182 O ILE 359 24.326 -7.355 61.843 1.00 32.83 ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5184 CA LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5185 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5187 CD1 LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5189 CD2 LEU 360 18.676 -9.901 62.188 1.00 39.70 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5193 CB ASN 361 22.050 -2.798 60.431 1.00 39.80 ATOM 5193 CB ASN 361 22.050 -2.798 60.431 1.00 39.80 ATOM 5193 CB ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 CD1 ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 CD1 ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 CD1 ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 CD1 ASN 361 22.119 -3.109 61.633 1.00 41.69 ATOM 5198 C ASN 361 18.630 -5.637 58.974 1.00 40.40 40 ATOM 5198 C ASN 361 18.630 -5.637 58.974 1.00 41.31 ATOM 5198 C ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5198 C ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5200 CA LYS 362 17.383 -3.604 59.555 1.00 40.39 ATOM 5200 CA LYS 362 17.383 -3.604 59.555 1.00 40.39 ATOM 5200 CA LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5200 CA LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5200 CA LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5200 CA LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5200 CA LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5200 CA LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5205 NZ LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5205 NZ LYS 362 17.383 -2.481 56.664 1.00 37.04 ATOM 5205 NZ LYS 362 17.385 -2.489 59.555 1.00 40.00 ATOM 5203 D NZ LYS 362 17.385 5	25										В
ATOM 5180 CD1 ILE 359 23.903 -7.152 62.984 1.00 33.89 ATOM 5181 C ILE 359 24.326 -7.355 61.843 1.00 32.83 ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5184 CA LEU 360 22.605 -7.249 62.211 1.00 39.23 ATOM 5185 CB LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CG LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5187 CD1 LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5188 CD LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5199 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5191 N ASN 361 20.786 -5.429 62.994 1.00 39.55 ATOM 5193 CB ASN 361 19.989 -4.286 60.413 1.00 39.80 ATOM 5193 CB ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5195 OD1 ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5195 ND2 ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.04 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.04 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.04 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.04 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.838 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.839 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.898 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.898 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.898 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS 362 17.898 -3.604 59.535 1.00 40.09 ATOM 5200 C LYS	23										В
ATOM 5181 C ILE 359 24.326 -7.355 61.843 1.00 33.89											. В
30 ATOM 5182 O ILE 359 24,326 -7.355 61.843 1.00 32.83 ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 36.27 ATOM 5186 CB LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5186 CB LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CG LEU 360 20.630 -9.122 60.240 1.00 44.94 35 ATOM 5188 CD LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5188 CD LEU 360 18.676 -9.901 62.188 1.00 45.24 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5193 CB ASN 361 19.989 -4.286 60.413 1.00 39.85 ATOM 5194 CG ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5196 ND2 ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5199 N LYS 362 17.838 -3.660 59.535 1.00 40.39 ATOM 5200 CA LYS 362 17.838 -3.660 59.535 1.00 40.39 ATOM 5201 CB LYS 362 17.283 -3.687 58.795 1.00 40.39 ATOM 5201 CB LYS 362 17.283 -3.687 58.795 1.00 40.39 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.283 -2.686 69.94 1.00 33.80 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 40.62 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5204 CE LYS 362 15.544 -4.838 59.222 1.00 40.02 ATOM 5209 MG G 2602 43.447 10.556 59.838 1.00 13.80 ATOM 5209 MG G 2602 43.447 10.556 59.838 1.00 12.39 ATOM 5209 MG G 2602 43.447 10.556 59.883 1.00 1.01 1.46 ATOM 5209 NG LYS 362 15.341 -5.705 58.378 1.00 40.02 ATOM 5204 CB LYS 362 15.944 -4.888 60.404 1.00 38.46 ATOM 5207 O LYS 362 15.484 -1.182 54.828 1.00 33.80 ATOM 5208 OXT LYS 362 15.444 -4.888 60.404 1.00 38.46 ATOM 5209 NG MG 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5206 C LYS 362 15.544 -4.888 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.664 -4.833 59.222 1.00 40.02 ATOM 5209 OX LYS 362 15.546 -5.830 59.855 1.00 19.46 ATOM 5209 OX LYS 362 15.946 -5.850 59.858 1.00 19.34 ATOM 5208 OX LYS 362 15.946 -5.85											В
ATOM 5183 N LEU 360 22.605 -7.080 63.256 1.00 36.27											В
ATOM 5184 CA LEU 360 21.597 -7.249 62.211 1.00 39.23 ATOM 5185 CB LEU 360 20.630 -8.381 62.583 1.00 42.29 ATOM 5186 CG LEU 360 19.497 -8.742 61.609 1.00 44.94 35 ATOM 5187 CDI LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5188 CD2 LEU 360 20.073 -9.122 60.240 1.00 44.70 ATOM 5189 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5190 O LEU 360 20.286 -5.429 62.994 1.00 39.75 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5192 CA ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5193 CB ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5194 CG ASN 361 22.050 -2.788 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.050 -2.788 60.350 1.00 41.69 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.67 ATOM 5198 O ASN 361 18.748 -4.575 59.575 1.00 40.40 45 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.31 ATOM 5200 CA LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5201 CB LYS 362 17.838 -3.604 59.535 1.00 40.38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 15.515 59.575 1.00 40.03 ATOM 5204 CE LYS 362 15.515 -2.535 55.151 1.00 35.58 ATOM 5206 C LYS 362 15.548 -1.182 54.828 1.00 33.80 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 40.02 ATOM 5209 MG MG 2602 43.447 10.556 59.833 1.00 11.01 ATOM 5209 MG MG 2602 43.447 10.556 59.833 1.00 11.06 ATOM 5209 MG MG 2602 43.447 10.556 59.833 1.00 12.39 ATOM 5209 MG MG 2600 44.598 7.110 60.307 1.00 18.59 ATOM 5240 O2B ADP 2600 44.598 7.110 60.307 1.00 18.59 ATOM 5240 O2B ADP 2600 44.598 7.110 60.307 1.00 18.59 ATOM 5240 O2B ADP 2600 44.598 7.110 60.307 1.00 18.59 ATOM 5240 O2B ADP 2600 44.598 7.110 60.307 1.00 18.59 ATOM 5240 O2B ADP 2600 44.598 7.110 60.307 1.00 18.59 ATOM 5240 O2B ADP 2600 44.598 7.110 60.307 1.00 18.59 ATOM 5240 O2B ADP 2600 44.990 5.607 6.595 57.824 1.00 22.53 ATOM 5240 O2B ADP 2600 45.933 7.683 57.885 1.00 19.34 ATOM 5240 O2B ADP 2600 44.990 5.608 59.185 1.00 19.34 ATOM 5240 O2B ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* A	20										В
ATOM 5185 CB LEU 360	30										В
ATOM 5186 CG LEU 360 19.497 -8.742 61.609 1.00 44.94											В
35 ATOM 5187 CDI LEU 360											В
ATOM 5188 CD2 LEU 360 18.676 -9.901 62.188 1.00 45.24 ATOM 5199 O LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5192 CA ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5193 CB ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5193 CB ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5194 CG ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.050 -2.798 60.350 1.00 41.21 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5197 C ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5198 O ASN 361 18.748 -4.575 59.575 1.00 40.40 45 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 16.572 -3.687 58.974 1.00 41.33 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 33.80 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5207 O LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5209 OIB ADP 2600 45.988 7.724 61.540 1.00 6.06 ATOM 5240 OZB ADP 2600 45.869 6.988 57.885 1.00 15.76 ATOM 5242 PA ADP 2600 45.869 6.988 57.895 1.00 14.04 ATOM 5242 PA ADP 2600 45.669 6.988 57.999 1.00 9.32 ATOM 5246 O									61.609	1.00 44.94	В
ATOM 5199 C LEU 360 20.800 -5.970 62.028 1.00 39.70 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 ATOM 5192 CA ASN 361 19.989 -4.286 60.413 1.00 39.80 ATOM 5193 CB ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5194 CG ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5197 C ASN 361 18.748 -4.575 55.575 1.00 40.40 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5199 N LYS 362 16.572 -3.687 58.974 1.00 41.33 ATOM 5200 CA LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.312 -2.553 55.151 1.00 40.39 ATOM 5202 CG LYS 362 17.312 -2.553 55.151 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5208 OXT LYS 362 15.248 1.182 54.828 1.00 33.80 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 40.02 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 40.02 ATOM 5239 DIB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 DIB ADP 2600 44.598 7.120 60.595 1.00 19.46 ATOM 5244 O2A ADP 2600 45.886 9.129 59.799 1.00 12.39 ATOM 5244 O2A ADP 2600 45.886 9.129 59.799 1.00 12.39 ATOM 5244 O2A ADP 2600 45.886 9.129 59.799 1.00 12.39 ATOM 5244 O2A ADP 2600 45.689 6.908 59.185 1.00 11.01 8.59 ATOM 5244 O2A ADP 2600 45.886 9.129 59.799 1.00 9.32 ATOM 5246 O5* ADP 2600 45.689 6.908 59.185 1.00 18.59 ATOM 5246 O5* ADP 2600 45.689 6.908 59.185 1.00 19.46 ATOM 5246 O5* ADP 2600 47.412 7.404 57.328 1.00 18.59 ATOM 5246 O5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5240 C2* ADP 2600 49.691 6.801 56.801 1.00 26.52 ATOM 5250 C2* ADP 2600 49.691 6.801 56.801 1.00 26.52 ATOM 5250 C2* ADP 2600 49.691 6.801 56.801 1.00 25.31 ATOM 5250 C2*	25										В
ATOM 5190 O LEU 360 20.286 -5.429 62.994 1.00 39.55 ATOM 5191 N ASN 361 20.710 -5.509 60.777 1.00 40.33 4.00 40.62 ATOM 5192 CA ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5193 CB ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 ODI ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5196 ND2 ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 41.33 ATOM 5198 O ASN 361 18.748 -4.575 59.575 1.00 40.40 41.33 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 41.69 ATOM 5200 CA LYS 362 16.537 58.974 1.00 41.33 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5201 CB LYS 362 17.283 -2.481 56.664 1.00 37.04 50.00 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 50.00 ATOM 5204 CE LYS 362 17.283 -2.481 56.664 1.00 37.04 50.00 ATOM 5205 NZ LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.548 -1.182 54.828 1.00 33.80 ATOM 5205 NZ LYS 362 15.548 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.548 -1.182 54.828 1.00 33.80 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 50.00 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 41.01 50.00 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 1.46 ATOM 5238 PB ADP 2600 45.869 9.195 1.00 9.47 ATOM 5238 PB ADP 2600 45.869 9.29 8.310 1.00 1.46 ATOM 5240 OZB ADP 2600 45.869 9.29 8.310 1.00 1.46 ATOM 5240 OZB ADP 2600 44.99 5.660 59.879 9.100 9.32	35	MOTA	5188	CD2	LEU	360	18.676	-9.901	62.188	1.00 45.24	В
40 ATOM 5191 N ASN 361 19.989 -4.286 60.413 1.00 39.80 ATOM 5193 CB ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5193 CB ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 OD1 ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 OD1 ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5196 ND2 ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 41.33 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.40 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 16.572 -3.687 58.974 1.00 41.33 ATOM 5201 CB LYS 362 16.572 -3.687 58.974 1.00 41.39 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.312 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.06 ATOM 5205 NZ LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.548 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.548 -1.182 54.828 1.00 33.80 ATOM 5207 O LYS 362 15.544 -4.833 59.222 1.00 40.02 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 028 ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 028 ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5240 028 ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5240 028 ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5246 05* ADP 2600 45.886 9.129 58.130 1.00 19.46 ATOM 5247 C5* ADP 2600 45.669 6.908 59.185 1.00 19.46 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5240 028 ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5245 03* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5245 03* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5245 03* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 03* ADP 2600 49.691 6.801 56.820 1.00 26.52 ATOM 5255 02* ADP 2600 49.698 7.905 53.303 1.00 27.28		ATOM	5189	С	LEU		20.800	-5.970	62.028	1.00 39.70	В
40 ATOM 5192 CA ASN 361 19.989 -4.286 60.413 1.00 39.80 ATOM 5193 CB ASN 361 22.050 -2.798 60.350 1.00 40.62 ATOM 5194 CG ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 OD1 ASN 361 22.893 -2.087 59.792 1.00 41.21 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 41.78 ATOM 5198 O ASN 361 18.748 -4.575 59.575 1.00 40.40 41.73 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 16.572 -3.687 58.974 1.00 41.33 ATOM 5201 CB LYS 362 16.572 -3.687 58.795 1.00 40.64 ATOM 5202 CG LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5205 NZ LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5206 C LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5206 C LYS 362 15.548 -1.182 54.828 1.00 33.80 ATOM 5208 OXT LYS 362 15.544 -4.833 59.222 1.00 40.02 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5239 DIB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 OZB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 OZB ADP 2600 44.98 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 44.98 5.627 60.595 1.00 9.32 ATOM 5242 PA ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5242 PA ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5244 OZA ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 49.591 6.801 56.820 1.00 22.53 ATOM 5248 C4* ADP 2600 49.591 6.801 56.820 1.00 22.53 ATOM 5249 O4* ADP 2600 49.591 6.801 56.620 1.00 24.49 ATOM 5247 C5* ADP 2600 49.591 6.801 56.620 1.00 24.49 ATOM 5249 O4* ADP 2600 49.591 6.801 56.620 1.00 24.13 ATOM 5251 O3* ADP 2600 49.591 6.801 56.620 1.00 24.13 ATOM 5252 C2* ADP 2600 49.594 7.992 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.594 7.992 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.594 7.995 55.501 1.00 26.52 ATOM 5253 O2* ADP 2600 49.594 7.995 55.3303 1.00 27.28		MOTA	5190	0	LEU	360	20.286	-5.429	62.994	1.00 39.55	В
40 ATOM 5193 CB ASN 361 20.865 -3.358 59.573 1.00 40.62 ATOM 5194 CG ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 DDI ASN 361 22.050 -2.798 60.350 1.00 41.61 ATOM 5196 ND2 ASN 361 22.093 -2.087 59.792 1.00 41.21 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 40.40 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 16.572 -3.687 58.795 1.00 40.39 ATOM 5201 CB LYS 362 16.572 -3.687 58.795 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5205 NZ LYS 362 15.544 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.544 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.544 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 4.64 ATOM 5238 PB ADP 2600 43.447 10.556 59.883 1.00 1.466 ATOM 5239 OTB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 OTB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 02B ADP 2600 44.998 5.627 60.595 1.00 9.47 ATOM 5241 03B ADP 2600 44.998 5.627 60.595 1.00 9.47 ATOM 5243 01A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5243 01A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5243 01A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5243 01A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 03A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5246 05* ADP 2600 49.591 6.801 56.820 1.00 24.49 ATOM 5248 C4* ADP 2600 49.591 6.801 56.820 1.00 24.49 ATOM 5248 C4* ADP 2600 49.591 6.801 56.698 1.00 22.53 ATOM 5249 04* ADP 2600 49.591 6.801 56.698 1.00 22.53 ATOM 5248 C4* ADP 2600 49.591 6.801 56.698 1.00 22.53 ATOM 5248 C4* ADP 2600 49.591 6.801 56.698 1.00 22.53 ATOM 5248 C4* ADP 2600 49.591 6.801 56.6098 1.00 22.53 ATOM 5248 C4* ADP 2600 49.591 6.801 56.604 1.00 22.53 ATOM 5251 03* ADP 2600 49.591 6.801 56.604 1.00 22.53 ATO		MOTA	5191	N	ASN	361	20.710	-5.509	60.777	1.00 40.33	В
ATOM 5194 CG ASN 361 22.050 -2.798 60.350 1.00 41.69 ATOM 5195 OD1 ASN 361 22.019 -3.109 61.633 1.00 41.21 ATOM 5196 ND2 ASN 361 22.119 -3.109 61.633 1.00 41.78 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 45 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 16.572 -3.687 58.795 1.00 40.39 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.544 -4.833 59.222 1.00 40.02 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5239 O1B ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 44.988 5.627 60.595 1.00 9.47 ATOM 5240 O2B ADP 2600 44.988 5.627 60.595 1.00 9.47 ATOM 5240 O2B ADP 2600 44.998 5.627 60.595 1.00 19.46 ATOM 5240 O2B ADP 2600 44.998 5.627 60.595 1.00 19.46 ATOM 5240 O2B ADP 2600 44.998 5.627 60.595 1.00 19.46 ATOM 5243 O1A ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5244 O2A ADP 2600 45.933 7.683 57.885 1.00 19.46 ATOM 5245 O3A ADP 2600 45.933 7.683 57.885 1.00 19.46 ATOM 5245 O3A ADP 2600 45.933 7.683 57.885 1.00 19.46 ATOM 5247 C5* ADP 2600 45.933 7.683 57.885 1.00 19.46 ATOM 5246 O5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 49.591 6.801 56.820 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 22.53 ATOM 5249 O4* ADP 2600 49.594 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.691 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.691 7.928 55.757 1.00 24.13 ATOM 5253 O2* ADP 2600 49.691 7.928 55.757 1.00 24.13 ATOM 5253 O2* ADP 2600 49.691 7.928 55.757 1.00 24.13	4.0	ATOM	5192	CA	ASN	361	19.989	-4.286	60.413	1.00 39.80	В
ATOM 5195 OD1 ASN 361	40	ATOM	5193	CB	ASN	361	20.865	-3.358	59.573	1.00 40.62	Ė
ATOM 5196 ND2 ASN 361		MOTA	5194	CG	ASN	361	22.050	-2.798	60.350	1.00 41.69	В
45 ATOM 5197 C ASN 361 18.748 -4.575 59.575 1.00 40.40 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5200 CA LYS 362 16.572 -3.687 58.795 1.00 40.39 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5206 C LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5206 C LYS 362 15.341 -5.705 58.378 1.00 41.01 5.00 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 41.01 5.00 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 OIB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 44.998 5.627 60.595 1.00 9.47 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 OIA ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5247 C5* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5248 C4* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.508 7.905 53.303 1.00 27.28		MOTA		OD1	ASN	361	22.893	-2.087	59.792	1.00 41.21	В
45 ATOM 5198 O ASN 361 18.630 -5.637 58.974 1.00 41.33 ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5201 CB LYS 362 16.572 -3.687 58.795 1.00 40.39 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 54.00 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5239 OIB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5243 OIA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 OIA ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 49.691 6.801 57.826 1.00 24.49 ATOM 5247 C5* ADP 2600 49.691 6.801 57.826 1.00 24.49 ATOM 5247 C5* ADP 2600 49.691 6.801 57.826 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 57.826 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 57.826 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 57.826 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 57.826 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5251 O3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA	5196	ND2	ASN	361	22.119	-3.109	61.633	1.00 41.78	В
ATOM 5199 N LYS 362 17.838 -3.604 59.535 1.00 40.64 ATOM 5201 CB LYS 362 16.572 -3.687 58.795 1.00 40.39 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 11.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 01B ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 02B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 03B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 01A ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5244 02A ADP 2600 45.866 9.129 58.130 1.00 18.59 ATOM 5246 05* ADP 2600 45.669 6.908 59.185 1.00 19.46 ATOM 5246 05* ADP 2600 45.669 6.908 59.185 1.00 19.34 ATOM 5246 05* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 04* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5249 04* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5250 C3* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5251 03* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 03* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.508 7.905 53.303 1.00 27.28	4 -	ATOM	5197	С	ASN	361	18.748	-4.575	59.575	1.00 40.40	ъ
ATOM 5200 CA LYS 362 16.572 -3.687 58.795 1.00 40.39 ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 O1B ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 44.998 5.627 60.595 1.00 9.47 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5242 PA ADP 2600 44.910 7.319 56.926 1.00 19.46 ATOM 5244 O2A ADP 2600 45.866 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.669 6.908 59.185 1.00 19.46 ATOM 5246 O5* ADP 2600 45.669 6.908 59.185 1.00 19.34 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.504 7.928 55.755 5.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.698 7.905 53.303 1.00 27.28	45	ATOM	5198	0	ASN	361	18.630	-5.637	58.974	1.00 41.33	В
ATOM 5201 CB LYS 362 16.811 -3.781 57.283 1.00 38.42 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 41.01 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 O1B ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 44.910 7.319 56.926 1.00 19.46 ATOM 5243 O1A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 49.699 5.805 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.699 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5251 O3* ADP 2600 49.594 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 50.670 8.755 55.611 1.00 25.52 ATOM 5252 C2* ADP 2600 50.670 8.755 55.611 1.00 25.52 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28		ATOM	5199	N	LYS	362	17.838	-3.604	59.535	1.00 40.64	В
50 ATOM 5202 CG LYS 362 17.283 -2.481 56.664 1.00 37.04 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5205 NZ LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 57.00 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 41.01 57.00 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5239 OIB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 OIB ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5241 O3B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 44.910 7.319 56.926 1.00 15.76 ATOM 5243 OIA ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5247 C5* ADP 2600 49.691 6.801 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 57.824 1.00 22.53 ATOM 5249 O4* ADP 2600 49.691 6.801 57.824 1.00 22.53 ATOM 5249 O4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.504 7.928 55.757 1.00 25.51 ATOM 5252 C2* ADP 2600 49.698 7.905 53.303 1.00 27.28		ATOM	5200	CA	LYS	362	16.572	-3.687	58.795	1.00 40.39	В
50 ATOM 5203 CD LYS 362 17.312 -2.553 55.151 1.00 35.58 ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 40.02 ATOM 5206 C LYS 362 15.341 -5.705 58.378 1.00 41.01 55 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5208 MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5240 O2B ADP		MOTA		CB			16.811	-3.781	57.283	1.00 38.42	В
ATOM 5204 CE LYS 362 15.915 -2.479 54.570 1.00 35.06 ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 O1B ADP 2600 44.598 7.724 61.540 1.00 6.06 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5241 O3B ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 O1A ADP 2600 45.933 7.683 57.885 1.00 19.46 ATOM 5244 O2A ADP 2600 45.866 9.129 58.130 1.00 18.59 ATOM 5246 O5* ADP 2600 45.669 6.908 59.185 1.00 19.46 ATOM 5246 O5* ADP 2600 45.669 6.908 59.185 1.00 19.34 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5248 C4* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5250 C3* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 50.670 8.755 55.611 1.00 25.52 ATOM 5252 C2* ADP 2600 50.670 8.755 55.611 1.00 25.52 ATOM 5252 C2* ADP 2600 50.670 8.755 55.611 1.00 25.52 ATOM 5252 C2* ADP 2600 49.698 7.905 53.303 1.00 27.28	~^	MOTA	5202	CG	LYS	362	17.283	-2.481	56.664	1.00 37.04	В
ATOM 5205 NZ LYS 362 15.248 -1.182 54.828 1.00 33.80 ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 ATOM 5208 OXT LYS 362 15.341 -5.705 58.378 1.00 41.01 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 O1B ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 O1A ADP 2600 44.910 7.319 56.926 1.00 19.46 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5246 O5* ADP 2600 45.886 9.129 58.130 1.00 19.34 ATOM 5247 C5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.51 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.21 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28	50	MOTA	5203	CD	LYS	362		-2.553	55.151	1.00 35.58	В
ATOM 5206 C LYS 362 15.654 -4.833 59.222 1.00 40.02 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 50.00 50.0		ATOM	5204	CE	LYS	362	15.915	-2.479	54.570	1.00 35.06	В
55 ATOM 5207 O LYS 362 15.341 -5.705 58.378 1.00 41.01 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 O1B ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 O1A ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.669 6.908 59.185 1.00 19.46 ATOM 5246 O5* ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5247 C5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.780 5.604 56.098 1.00 22.53 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.34 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 25.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA		NZ	LYS	362	15.248	-1.182	54.828	1.00 33.80	В
55 ATOM 5208 OXT LYS 362 15.244 -4.848 60.404 1.00 38.46 ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5240 O2B ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5241 O3B ADP 2600 43.494 7.932 59.799 1.00 9.47 ATOM 5242 PA ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 19.46 ATOM 5243 O1A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A AD		MOTA			LYS	362				1.00 40.02	В
ATOM 5209 MG MG 2602 43.447 10.556 59.883 1.00 1.46 ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 O1B ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 O1A ADP 2600 44.910 7.319 56.926 1.00 19.46 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5246 O5* ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5247 C5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.51 ATOM 5252 C2* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA	5207	0	LYS	362	15.341	-5.705	58.378		В
ATOM 5238 PB ADP 2600 44.598 7.110 60.307 1.00 12.39 ATOM 5239 018 ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5241 038 ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 44.910 7.319 56.926 1.00 15.76 ATOM 5243 01A ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5244 02A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 03A ADP 2600 45.669 6.908 59.185 1.00 18.59 ATOM 5247 05. ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 05. ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 04* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 03* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 02* ADP 2600 49.698 7.905 53.303 1.00 27.28	22	MOTA		OXT	LYS	362	15.244	-4.848	60.404	1.00 38.46	В
ATOM 5239 01B ADP 2600 45.185 7.724 61.540 1.00 6.06 ATOM 5240 02B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 03B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 01A ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5244 02A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 03A ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5246 05* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 49.691 6.801 56.820 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5251 03* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 03* ADP 2600 49.154 7.243 54.456 1.00 25.51 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 02* ADP 2600 49.698 7.905 53.303 1.00 27.28					MG		43.447			1.00 1.46	
60 ATOM 5240 O2B ADP 2600 44.098 5.627 60.595 1.00 9.47 ATOM 5241 O3B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 O1A ADP 2600 45.933 7.683 57.885 1.00 19.46 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5246 O5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 22.53 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5250 C3* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5251 O3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA					44.598	7.110	60.307	1.00 12.39	ADP
60 ATOM 5241 03B ADP 2600 43.494 7.932 59.799 1.00 9.32 ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 01A ADP 2600 44.910 7.319 56.926 1.00 19.46 ATOM 5244 02A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 03A ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5246 05* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 48.489 6.585 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 04* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 03* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 02* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA		01B	ADP	2600	45.185	7.724	61.540	1.00 6.06	ADP
ATOM 5242 PA ADP 2600 45.933 7.683 57.885 1.00 15.76 ATOM 5243 01A ADP 2600 44.910 7.319 56.926 1.00 19.46 ATOM 5244 02A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 03A ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5246 05* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 48.489 6.585 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 04* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 03* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 02* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA	5240	02B	ADP	2600	44.098	5.627	60.595	1.00 9.47	ADP
ATOM 5243 O1A ADP 2600 44.910 7.319 56.926 1.00 19.46 ATOM 5244 O2A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 O3A ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5246 O5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 48.489 6.585 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28	60	MOTA	5241	03B	ADP	2600	43.494	7.932	59.799	1.00 9.32	ADP
ATOM 5244 02A ADP 2600 45.886 9.129 58.130 1.00 18.59 ATOM 5245 03A ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5246 05* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 22.53 ATOM 5249 04* ADP 2600 49.780 5.604 56.098 1.00 24.49 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 03* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 02* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA	5242	PA	ADP	2600	45.933	7.683	57.885	1.00 15.76	ADP
ATOM 5245 O3A ADP 2600 45.669 6.908 59.185 1.00 14.04 ATOM 5246 O5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 48.489 6.585 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28		ATOM	5243	01A	ADP	2600	44.910	7.319	56.926	1.00 19.46	ADP
65 ATOM 5246 O5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 48.489 6.585 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28		ATOM	5244	02A	ADP	2600	45.886	9.129	58.130	1.00 18.59	ADP
65 ATOM 5246 O5* ADP 2600 47.412 7.404 57.328 1.00 19.34 ATOM 5247 C5* ADP 2600 48.489 6.585 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28	<i>-</i> -	ATOM	5245								ADP
ATOM 5247 C5* ADP 2600 48.489 6.585 57.824 1.00 22.53 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28	65	MOTA	5246	05*	ADP	2600		7.404			ADP
70 ATOM 5248 C4* ADP 2600 49.691 6.801 56.820 1.00 24.49 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28											ADP
70 ATOM 5249 O4* ADP 2600 49.780 5.604 56.098 1.00 26.34 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28											ADP
70 ATOM 5250 C3* ADP 2600 49.504 7.928 55.757 1.00 24.13 ATOM 5251 O3* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28			5249	04*	ADP				56.098		ADP
/U ATOM 5251 03* ADP 2600 50.670 8.755 55.611 1.00 26.52 ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 02* ADP 2600 49.698 7.905 53.303 1.00 27.28			5250		ADP				55.757		ADP
ATOM 5252 C2* ADP 2600 49.154 7.243 54.456 1.00 25.11 ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28	70	ATOM		03*	ADP						ADP
ATOM 5253 O2* ADP 2600 49.698 7.905 53.303 1.00 27.28		MOTA	5252			2600				1.00 25.11	ADP
		MOTA				2600	49.698				ADP
		MOTA	5254	C1*	ADP	2600	49.652		54.676	1.00 26.94	ADP

	MOTA	5255	N9	ADP	2600	48.736	4.765	54.191	1.00 27.64	ADP
	ATOM	5256	C8	ADP	2600	47.767	4.193	54.941	1.00 26.96	ADP
	ATOM	5257	N7	ADP	2600	47.150	3.292	54.228	1.00 29.21	ADP .
_	ATOM	5258	C5	ADP	2600	47.690	3.269	53.027	1.00 29.55	ADP
5	ATOM	5259	C6	ADP	2600	47.466	2.525	51.857	1.00 29.68	ADP
	ATOM .	5260	N6	ADP	2600	46.495	1.606	51.861	1.00 29.43	ADP
	MOTA	5261	N1	ADP	2600	48.250	2.751	50.704	1.00 30.06	ADP
	MOTA	5262	C2	ADP	2600	49.252	3.696	50.678	1.00 29.27	ADP
	ATOM	5263	N3	ADP	2600	49.466	4.411	51.827	1.00 29.94	ADP
10	MOTA	5264	C4	ADP	2600	48.711	4.230	52.991	1.00 28.23	ADP
	ATOM	5291	C1	4-2A	1	42.197	14.937	49.097	1.00 25.59	4-2A
	MOTA	5292	C2	4-2A	1	41.920	14.433	47.714	1.00 25.74	4-2A
	ATOM	5293	C3	4-2A	1	41.044	15.120	46.829	1.00 26.03	4-2A
	ATOM	5294	C4	4-2A	1	40.929	14.774	45.500	1.00 26.67	4-2A
15	ATOM	5295	C5	4-2A	1	41.663	13.715	44.991	1.00 25.62	4-2A
	MOTA	5296	C6	4-2A	1	42.514	12.931	45.817	1.00 25.53	4-2A
	MOTA	5297	C7	4-2A	1	42.617	13.291	47.201	1.00 25.82	4-2A
	MOTA	5298	012	4-2A	1	43.246	11.914	45.291	1.00 25.59	4-2A
	MOTA	5299	C14	4-2A	1	40.974	14.917	49.926	1.00 26.54	4-2A
20	MOTA	5300	C15	4-2A	1	40.461	16.085	50.528	1.00 26.66	4-2A
	ATOM	5301	C16	4-2A	1	41.255	17.420	50.551	1.00 26.17	4-2A
	ATOM ·	5302	C17	4-2A	1	42.265	17.452	49.404	1.00 26.31	4-2A
	ATOM	5303	N18	4-2A	1	42.979	16.179	49.355	1.00 26.30	4-2A
	MOTA	5304	C22	4-2A	1	43.422	18.425	49.565	1.00 25.84	4-2A
25	ATOM	5305	N23	4-2A	1	44.551	17.713	49.505	1.00 25.90	4-2A
	MOTA	5306	C24	4-2A	1	44.289	16.370	49.394	1.00 26.52	4-2A
	MOTA	5307	N26	4-2A	1	40.109	13.877	50.027	1.00 26.97	4-2A
	MOTA	5308	C27	4-2A	1	38.991	14.325	50.732	1.00 26.51	4-2A
~~	MOTA	5309		4-2A	1	39.211	15.740	51.093	1.00 27.62	4-2A
30	ATOM	5310	C29	4-2A	1	37.745	13.725	51.140	1.00 26.04	4-2A
	MOTA	5311		4-2A	1	36.783	14.431	51.909	1.00 26.80	4-2A
	MOTA	5312		4-2A	1	37.035	15.782	52.312	1.00 27.44	4-2A
	MOTA	5313		4-2A	1	38.217	16.439	51.892	1.00 27.46	4-2A
~~	ATOM	5314	037	4-2A	1	43.236	19.647	49.683	1.00 24.48	4-2A
35	MOTA	5315		4-2A	1	45.096	15.436	49.375	1.00 27.32	4-2A
	MOTA	5316	C39	4-2A	1	45.831	18.372	49.744	1.00 25.80	4-2A
	END									

TABLE 5

```
40
       REMARK
                 1 kin_16dpb molecule B
       REMARK r= 0.2114 free_r= 0.2639
       REMARK rmsd bonds= 0.006712 rmsd angles= 1.32262
       REMARK B rmsd for bonded mainchain atoms= 1.570 target= 1.5
45
       REMARK B rmsd for bonded sidechain atoms= 2.570 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.729 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.936 target= 2.5
       REMARK sg= P2(1)2(1)2(1) a= 69.48 b= 79.54 c= 158.98 alpha= 90. beta= 90. gamma= 90.
       REMARK reflection file= k2a.cv
50
       REMARK B-correction resolution: 6.0 - 2.5
REMARK FILENAME="kin_16dpb.pdb"
ATOM 788 N GLU 116 39.151
                                              39.151 9.227
39.430 10.450
39.921 11.534
                                                                  52.663
51.915
52.868
                                                                           1.00
                                   116
116
                                                                                   8.87
                                                                                                В
                       CA GLU
       ATOM
                 789
                                                                                   8.17
                                                                            1.00
                                                                                                В
       ATOM
                 790
                       CB
                           GLU
                                   116
                                                                            1.00 8.92
1.00 12.15
                                                                                                B
55
       ATOM
                 791
                       CG
                                   116
                                              38.920
                                                        11.894
                                                                  53.939
                            GLU
                                                                                                В
       ATOM
                 792
                       CD
                            GLU
                                   116
                                               39.349
                                                        13.091
                                                                  54.738
                                                                            1.00 15.35
       MOTA
                 793
                       OE1 GLU
                                   116
                                               40.362
                                                        13.717
                                                                  54.354
                                                                            1.00 17.99
                                                                                                В
       ATOM
                 794
                       OE2 GLU
                                   116
                                              38.678
                                                        13.410
                                                                  55.737
                                                                            1.00 15.94
                                                                                                В
       MOTA
                 795
                            GLU
                                   116
                                               40.426
                                                        10.321
                                                                  50.784
                                                                            1.00
                                                                                  8.20
60
       MOTA
                 796
                       0
                            GLU
                                   116
                                               40.163
                                                        10.736
                                                                  49.657
                                                                            1.00
                                                                                    4.89
       MOTA
                 797
                            GLY
                                   117
                                               41.577
                                                         9.744
                                                                  51.097
                                                                            1.00
       MOTA
                 798
                       CA
                            GLY
                                   117
                                               42.619
                                                         9.608
                                                                  50.104
                                                                            1.00 10.26
       MOTA
                 799
                            GLY
                                   117
                                               43.531
                                                        10.819
                                                                  50.183
                                                                            1.00 11.18
       ATOM
                 800
                       0
                            GLY
                                   117
                                               43.289
                                                        11.751
                                                                  50.951
                                                                            1.00 10.98
                                                                                                В
65
       MOTA
                 801
                       N
                            GLU
                                   118
                                               44.590
                                                        10.813
                                                                  49.389
                                                                            1.00 13.18
       ATOM
                 802
                                   118
                                               45.531
                       CA
                            GLU
                                                        11.922
                                                                  49.386
                                                                            1.00 14.36
                                                                                                В
                                   118
118
118
118
       ATOM
                 803
                           GLU
GLU
                                               46.849
                       CB
                                                        11.498
                                                                  50.043
                                                                            1.00 15.18
                                                                                                В
       ATOM
                 804
                                                                  51.363
51.970
51.215
                       CG
                                               46.685
                                                        10.756
                                                                            1:00 21.23
                                                                                                В
                 805
                            GLU
                                                        10.310
9.845
       MOTA
                       CD
                                                                            1.00 24.46
                                               48.014
                                                                                                B
70
                                               48.894
       ATOM
                 806
                       OE1 GLU
                                                                            1.00 27.49
                                                                                                В
                 807
       MOTA
                       OE2 GLU
                                               48.177 10.413
                                                                  53.205
                                                                            1.00 26.10
                                   118
```

	ATOM	808	С	GLU	118	45.770	12.281	47.933	1.00 13.80	В
	MOTA	809	0	GLU	118	45.126	11.734	47.041	1.00 14.44	В
	ATOM	810	N	ARG	119	46.689	13.201	47.685	1.00 13.24	В
_	MOTA	811	CA	ARG	119	46.984	13.568	46.315	1.00 14.66	В
5	MOTA	812	CB	ARG	119	47.120	15.088	46.167	1.00 12.36	В
	MOTA	813	CG	ARG	119	45.879	15.905	46.518	1.00 11.10	В
	MOTA	814	CD	ARG	119	44.628	15.371	45.842	1.00 12.06	В
	MOTA	815	NE	ARG	119	44.829	15.087	44.422	1.00 13.81	В
	ATOM	816	CZ	ARG	119	44.750	15.992	43.451	1.00 14.81	В
10	MOTA	817	NH1	ARG	119	44.464	17.257	43.742	1.00 13.37	B
	ATOM	818		ARG	119	44.964	15.632	42.189	1.00 11.75	В
	ATOM	819	С	ARG	119	48.288	12.911	45.889	1.00 16.73	В
	MOTA	820	ŏ	ARG	119	49.253	12.857	46.662	1.00 17.59	В
`	MOTA	879	N	TRP	127	42.371	15.847	40.233	1.00 18.06	В
15	ATOM	880	CA	TRP	127	41.717	15.171	41.335	1.00 16.78	В
	ATOM	881	CB	TRP	127	40.912	16.167	42.178	1.00 14.46	B
	ATOM	882	CG	TRP	127	39.646	16.618	41.539	1.00 10.93	В
	MOTA	883		TRP	127	38.365	15.996	41.664	1.00 8.71	В
	ATOM	884		TRP	127	37.452	16.770	40.915	1.00 9.40	В
20	ATOM	885		TRP	127	37.901	14.857	42.334	1.00 7.23	В
	ATOM	886		TRP	127	39.474	17.709	40.738	1.00 10.58	В
	MOTA	887		TRP	127	38.153	17.810	40.361	1.00 8.88	В
	ATOM	888		TRP	127	36.095	16.446	40.820	1.00 9.55	В.
	ATOM	889		TRP	127	36.545	14.526	42.242	1.00 9.73	B
25	ATOM	890		TRP	127	35.659	15.324	41.488	1.00 11.69	В
	MOTA	891	c	TRP	127	40.828	14.002	40.941	1.00 17.94	В
	ATOM	892	ŏ	TRP	127	40.817	12.978	41.621	1.00 18.94	В
	MOTA	911	N	ASP	130	43.130	10.872	40.183	1.00 18.67	В
	MOTA	912	CA	ASP	130	44.174	10.489	41.121	1.00 17.72	В
30	ATOM	913	CB	ASP	130	44.298	11.534	42.229	1.00 15.27	В
	ATOM	914	CG	ASP	130	45.675	11.545	42.859	1.00 16.56	В
	MOTA	915		ASP	130	46.157	10.473	43.285	1.00 15.04	В
•	ATOM	916		ASP	130	46.277	12.634	42.930	1.00 16.73	В
	ATOM	917	c	ASP	130	43.921	9.115	41.733	1.00 16.61	В
35	ATOM	918	ō	ASP	130	42.931	8.905	42.430	1.00 19.40	В
	ATOM	926	N	LEU	132	45.069	7.791	44.240	1.00 15.09	В
	MOTA	927	CA	LEU	132	45.118	7.772	45.703	1.00 13.40	В
	MOTA	928	СВ	LEU	132	46.379	8.487	46.227	1.00 10.29	В
	ATOM	929	CG	LEU	132	47.765	7.870	45.930	1.00 10.29	
40	ATOM	930		LEU	132	48.877	8.709	46.609	1.00 8.52	B B
	ATOM	931		LEU	132	47.829	6.414	46.429	1.00 11.00	В
	MOTA	932	c	LEU	132	43.858	8.395	46.310	1.00 12.82	В
	ATOM	933	ŏ	LEU	132	43.719	8.473	47.534	1.00 12.02	В
	ATOM	934	N	ALA	133	42.936	8.833	45.457	1.00 12.47	В
45	MOTA	935	CA	ALA	133	41.681	9.414	45.936	1.00 12.78	В
	MOTA	936	CB	ALA	133	40.826	9.884	44.755	1.00 11.66	В
	ATOM	937	Č	ALA	133	40.928	8.356	46.742	1.00 13.76	В
	ATOM	938	ŏ	ALA	133	40.991	7.163	46.431	1.00 13.92	В
	ATOM	939	N	GLY	134	40.217	8.798	47.776	1.00 14.68	В
50	ATOM	940	CA	GLY	134	39.483	7.870	48.619	1.00 13.15	В
	MOTA	941	C	GLY	134	38.016	7.752	48.262	1.00 14.05	В
	MOTA	942	0	GLY	134	37.574	8.262	47.228	1.00 12.84	В
	MOTA	951	N	ILE	136	35.223	9.141	49.530	1.00 10.60	B
	MOTA	952	CA	ILE	136	34.466	10.377	49.379	1.00 10.62	В
55	MOTA	953	CB	ILE	136	34.843	11.386	50.482	1.00 10.47	В
	ATOM	954	CG2		136	34.175	12.721	50.231	1.00 8.18	В
	ATOM	955	CG1		136		10.847	51.839	1.00 10.73	B
	ATOM	956	CD1		136	34.760	11.746	53.047	1.00 13.23	В
	ATOM	957	С	ILE	136	34.553	11.030	47.995	1.00 11.05	В
60 ·	MOTA	958	ō	ILE	136	33.531	11.296	47.373	1.00 10.67	В
	ATOM	959	N	PRO	137	35.765	11.303	47.492	1.00 11.64	В
	ATOM	960	CD	PRO	137	37.100	11.313	48.114	1.00 11.30	В
	ATOM	961	CA	PRO	137	35.793	11.924	46.162	1.00 11.06	В
	ATOM	962	СВ	PRO	137	37.237	12.410	46.031	1.00 10.03	
65	ATOM	963	CG	PRO	137	38.002	11.469	46.911	1.00 10.03	B B
	ATOM	964	c	PRO	137	35.369	10.997	45.019	1.00 11.03	В
	MOTA	965	Ö	PRO	137	34.867	11.455	43.989	1.00 11.71	В
	ATOM	1145	N	LEU	160	29.446	18.027	56.397	1.00 11.71	B
	ATOM	1146	CA	LEU	160	30.595	17.478	57.077	1.00 13.18	В
70	ATOM	1147		LEU	160	31.883	18.025	56.470	1.00 13.18	В
	ATOM	1148		LEU	160	33.175	17.477	57.068	1.00 13.62	В
	ATOM	1149	CD1		160	33.056	15.961	57.243	1.00 13.82	В
	ATOM	1150	CD2		160	34.343	17.846	56.166	1.00 13.33	В
						222	1	20.100	13.33	ь

	MOTA	1151	С	LEU	160	30.492	17.857	58.543	1.00 13.90	В
	ATOM	1152	0	LEU	160	30.883	18.956	58.947	1.00 11.88	В .
	ATOM	1564	N	TYR	211	35.581	19.271	44.173	1.00 18.55	· B
5	MOTA	1565	CA	TYR	211	36.924	19.418	44.731	1.00 18.51	В
J	MOTA	1566	CB	TYR	211	37.994	19.405	43.637	1.00 15.05	В
	ATOM	1567	CG	TYR	211	39.385	19.255	44.201	1.00 14.52	В
	MOTA	1568	CD1	TYR	211	39.721	18.153	44.981	1.00 15.06	В
	MOTA	1569	CE1	TYR	211	40.989	18.023	45.540	1.00 14.43	В
	MOTA	1570	CD2	TYR	211	40.359		43.988	1.00 13.72	В
10	ATOM	1571	CE2		211	41.629	20.112	44.541	1.00 12.86	В.
	MOTA	1572	CZ	TYR	211	41.937	19.003	45.316	1.00 13.41	• В
	MOTA	1573	OH	TYR	211	43.192	18.863	45.864	1.00 13.57	В
	MOTA	1574	C	TYR	211	37.044	20.683	45.575	1.00 19.47	B
	MOTA	1575	. 0	TYR	211	37.56 7	20.640	46.688	1.00 21.09	В
15	MOTA	1593	N	LEU	214	35.512	20.128	48.935	1.00 13.24	. В
	ATOM	1594	CA	LEU	214	36.304	19.274	49.805	1.00 13.61	В
	ATOM	1595	CB	LEU	214	36.778	18.022	49.055	1.00 11.20	. В
	ATOM	1596	CG	LEU	214	35.695	17.141	48.423	1.00 12.16	В
20	MOTA	1597	CD1		214	36.340	15.933	47.756	1.00 10.83	В
20	MOTA	1598	CD2		214	34.703	16.686	49.485	1.00 11.84	В
	ATOM	1599	С	LEU	214	37.503	20.063	50.332	1.00 14.64	В
	MOTA	1600	0	LEU	214	37.903	19.885	51.476	1.00 16.56	В
	MOTA	1601	N	GLU	215	38.065	20.946	49.506	1.00 16.42	В
	ATOM	1602	CA	GLU	215	39.216	21.748	49.930	1.00 18.40	В
25	MOTA	1603		GLU	215	39.764	22.595	48.781	1.00 18.89	• В
		1604							1.00 21.62	
	MOTA			GLU	215	40.428	21.819	47.673		В
	MOTA	1605		GLU	215	40.989	22.739	46.598	1.00 25.34	В
	MOTA	1606	OE1		215	42.227	22.957	46.572	1.00 24.25	В
20	MOTA	1607	QE2	GLU	215	40.182	23.256	45.788	1.00 24.35	В
30	MOTA	1608	С	GLU	215	38.856	22.676	51.077	1.00 17.37	В
	MOTA	1609	0	GLU	215	39.600	22.779	52.053	1.00 17.62	В
	ATOM	1619		GLY	217	36.574	22.385	53.343	1.00 17.13	В
	ATOM	1620		GLY	217	36.448	21.651	54.586	1.00 16.36	B
	ATOM	1621		GLY	217	37.821	21.367	55.173	•	. В
35									1.00 16.18	
"	MOTA	1622		GLY	217	38.044	21.542	56.378	1.00 15.76	В.
	MOTA	1623		ALA	218	38.746	20.934	54.322	1.00 15.35	В
	MOTA	1624		ALA	218	40.105	20.629	54.763	1.00 15.51	В
	MOTA	1625	CB	ALA	218	40.923	20.071	53.596	1.00 14.52	В
.:_	ATOM	1626	С	ALA	218	40.806	21.849	55.356	1.00 14.85	В
40	ATOM	1627	0	ALA	218	41.470	21.745	56.386	1.00 15.80	В
-	ATOM	1642		ARG	221	39.496	22.571	58.714	1.00 13.46	В
	ATOM	1643		ARG	221	39.917	21.498	59.606	1.00 14.10	В
	ATOM	1644		ARG	221	39.866	20.171	58.853		В
									1.00 13.82	
45	ATOM	1645		ARG	221	39.982	18.949	59.723	1.00 18.08	В
43	MOTA	1646		ARG	221	39.939	17.690	58.874	1.00 19.00	В
	MOTA	1647	NE	ARG	221	38.585	17.167	58.725	1.00 18.62	В
	ATOM	1648	CZ	ARG	221	38.226	16.296	57.788	1.00 20.44	В
	MOTA	1649	NH1	ARG	221	39.122	15.860	56.905	1.00 20.22	В
	ATOM	1650	NH2	ARG	221	36.980	15.839	57.751	1.00 16.95	В
50	ATOM	1651		ARG	221	41.331	21.780	60.137	1.00 14.31	В
	MOTA	1652		ARG	221	41.669	21.408	61.271	1.00 14.60	В
	ATOM	1777	-	PHE	239	30.844	12.531	56.963		В
									1.00 10.36	
	ATOM	1778		PHE	239	30.590	13.199	55.695	1.00 10.45	В
E E	MOTA	1779		PHE	239	31.785	13.041	54.753	1.00 10.20	В
55	ATOM	1780		PHE	239	31.691	13.879	53.513	1.00 7.76	. В
	MOTA	1781	CD1	PHE	239	30.822	13.533	52.479	1.00 7.06	В
	ATOM	1782	CD2	PHE	239	32.466	15.026	53.386	1.00 6.02	В
	MOTA	1783	CE1		239	30.729	14.329	51.327	1.00 7.31	В
	ATOM	1784	CE2		239	32.384	15.829	52.242	1.00 6.13	. В
60	ATOM	1785		PHE	239	31.516	15.483	51.210	1.00 5.13	В
00										
	ATOM	1786		PHE	239	29.350	12.555	55.085	1.00 12.53	В
	ATOM	1787		PHE	239	29.360	11.369	54.734	1.00 12.06	В
	MOTA	2624		MG	2602	43.714	10.353	59.884	1.00 13.44	
	ATOM	2625	PB	ADP	2600	44.677	7.176	60.125	1.00 9.41	ADP
65	ATOM	2626	01B		2600	45.207	7.814	61.350	1.00 10.96	ADP
	ATOM	2627	02B		2600	44.169	5.685	60.429	1.00 12.45	ADP
	ATOM	2628	03B		2600	43.584	7.969	59.545	1.00 12.43	ADP
	ATOM	2629		ADP	2600	46.112	7.788	57.787	1.00 12.25	ADP
70	MOTA	2630	01A		2600	45.124	7.466	56.774	1.00 14.66	ADP
70	MOTA	2631	02A		2600	46.054	9.225	58.059	1.00 14.40	ADP
	ATOM	2632	O3A		2600	45.825	7.002	59.093	1.00 9.50	ADP
	MOTA	2633	05*	ADP	2600	47.568	7.490	57.279	1.00 16.91	ADP
	ATOM	2634	C5*		2600	48.603	6.677	57.812	1.00 18.22	ADP
						,				

	ATOM	2635	C4*	ADP	2600	49.807	6.826	56.807	1.00 21.00	ADP
	ATOM	2636	04*	ADP	2600	49.837	5.609	56.073	1.00 23.65	ADP
	ATOM	2637	C3*	ADP	2600	49.662	7.936	55.733	1.00 20.88	ADP
_	ATOM	2638	03*	ADP	2600	50.883	8.668	55.538	1.00 23.91	ADP
5	MOTA	2639	C2*	ADP	2600	49.227	7.250	54.452	1.00 21.72	ADP
	ATOM	2640	02*	ADP	2600	49.726	7.910	53.286	1.00 24.74	ADP
	ATOM	2641	C1*	ADP	2600	49.720	5.835	54.648	1.00 22.48	ADP
	ATOM	2642	N9	ADP	2600	48.789	4.775	54.145	1.00 22.01	ADP
	MOTA	2643	C8	ADP	2600	47.775	4.231	54.861	1.00 22.26	ADP
10	ATOM	2644	N7	ADP	2600	47.163	3.322	54.140	1.00 24.15	ADP
	MOTA	2645	·C5	ADP	2600	47.742	3.257	52.980	1.00 24.22	ADP
	MOTA	2646	C6	ADP	2600	47.552	2.498	51.838	1.00 25.28	ADP
	ATOM	2647	N6	ADP	2600	46.577	1.596	51.801	1.00 26.60	ADP
	ATOM	2648	N1	ADP	2600	48.372	2.684	50.738	1.00 28.22	ADP
15	ATOM	2649	C2	ADP	2600	49.388	3.599	50.736	1.00 27.91	ADP
	ATOM	2650	N3	ADP	2600	49.583	4.338	51.852	1.00 25.85	ADP
	ATOM	2651	C4	ADP	2600	48.803	4.199	52.972	1.00 23.75	ADP
	MOTA	2879	C1	5-2b	1	40.179	14.530	46.990	1.00 27.45	5-2b
~~	MOTA	2880	C2	5-2ⴆ	1	41.169	13.921	47.825	1.00 31.74	5-2b
20	MOTA	2881	C3	5-2b	1	42.197	13.109	47.246	1.00 26.68	5-2b
	MOTA	2882	C4	5-2b	. 1	42.197	12.949	45.832	1.00 25.21	5-2b
	MOTA	2883	C5	5-2b	1	41.213	13.549	44.997	1.00 25.57	5-2b
	MOTA	2884	C6	5-2b	1	40.174	14.358	45.564	1.00 26.52	5-2b
25	MOTA	2885	C7	5-2b	1	41.159	14.149	49.287	1.00 39.17	5-2b
25	MOTA	2886	И8	5-2b	1	40.043	13.644	50.068	1.00 32.24	5-2b
	MOTA	2887	C9	5-2b	1	39.077	14.446	50.550	1.00 31.10	5-2b
	MOTA	2888		5-2b	1	39.335	15.753	50.627	1.00 35.90	5-2b
	MOTA	2889		5-2b	1	40.586	16.353	50.204	1.00 43.34	5-2b
20	ATOM	2890		5-2b	1	41.575	15.550	49.725	1.00 51.84	5-2b
30	ATOM	2891	013		1	43.103	12.325	45.318	1.00 22.27	5-2b
	MOTA	2892	C14		1	43.049	15.950	49.559	1.00 69.59	5-2b
	MOTA	2893	015		1	43.510	17.255	49.536	1.00102.78	5-2b
	MOTA	2894		5-2b	1	44.900	17.802	49.405	1.00 94.24	5-2b
35 ⁻	MOTA	2895	C17		1	44.910	19.338	49.209	1.00 96.86	5-2b
22	MOTA	2896	C18	5-2b	1	40.562	17.864	50.356	1.00 41.39	5-2b
	ATOM	2897		5-2b	1	43.806	15.026	49.427	1.00 72.75	5-2b
	MOTA	2898	S20	5-2b	1	37.588	13.867	51.069	1.00 18.63	5-2b
	D) III									

WHAT IS CLAIMED IS:

5

10

1. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table $1 \pm$ the root mean square deviation from the conserved backbone atoms of not more than about 2 Å.

- 2. The crystallized complex of Claim 1, wherein the relative structural coordinates of the amino acid residues are as set forth in Table $1 \pm$ the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.
- 3. The crystallized complex of Claim 1, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).
- 4. A crystallized complex of KSP and a ligand thereof,
 20 wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table 2 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.
- 5. The crystallized complex of Claim 4, wherein the relative structural coordinates of the amino acid residues are as set forth in Table 2 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.
- 6. The crystallized complex of Claim 4, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).

7. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table $3 \pm$ the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.

5

8. The crystallized complex of Claim 7, wherein the relative structural coordinates of the amino acid residues are as set forth in Table $3 \pm$ the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.

10

15

20

25

- 9. The crystallized complex of Claim 7, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).
- 10. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table $4 \pm$ the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.
- 11. The crystallized complex of Claim 10, wherein the relative structural coordinates of the amino acid residues are as set forth in Table $4 \pm$ the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.
- 12. The crystallized complex of Claim 10, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).
- 13. A ligand binding site of a KSP protein comprising the relative structural coordinates set forth in Table $5 \pm$ the root mean square

WO 2004/004652

deviation from the backbone atoms of said amino acids is not more than about 2 Å.

- 14. The ligand binding site of a KSP protein according to
 5 Claim 13 comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids is not more than about 0.5 Å.
- Claim 13 comprising the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) as set forth in a table selected from a group consisting of Tables 1, 2, 3 and 4, ± the root mean square deviation from the backbone atoms of said amino acids is not more than about 2 Å.
 - 16. An agent which binds to the ligand binding site of Claim 13, wherein said agent is an inhibitor of KSP function, or a pharmaceutically acceptable salt thereof.

20

- 17. A composition comprising: (a) an agent according to Claim 16; and (b) a pharmaceutically acceptable carrier.
- 18. An agent, or a pharmaceutically acceptable salt
 25 thereof, which binds to five or more of the KSP amino acid residues selected from the group consisting of 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), wherein said agent is an inhibitor of KSP function.

- 19. A method for identifying an agent that interacts with a ligand binding site of human KSP, comprising the steps of:
 - (a) determining a ligand binding site of KSP from a threedimensional model of the KSP binding site as set forth in

Table 5, \pm the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; and

(b) performing computer fitting analysis to identify an agent which interacts with said ligand binding site.

5

25

- 20. A method for identifying an agent that interacts with a ligand binding site of human KSP, comprising the steps of:
- (a) determining a ligand binding site of KSP from a three-dimensional model of KSP using the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) as set forth in a Table selected from the group of Tables 1, 2, 3 and 4, ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; and
 - (b) performing computer fitting analysis to identify an agent which interacts with said ligand binding site.
- 20 21. A method for identifying a potential inhibitor of KSP function, comprising the steps of:
 - (a) obtaining a three-dimensional model of a KSP binding site wherein said model contains the relative structural coordinates of the ligand binding site of KSP from a threedimensional model of the ligand binding site as set forth in Table 5, ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å;
 - (b) employing said three-dimensional model to design or select a potential inhibitor; and
 - (c) synthesizing or obtaining said potential inhibitor.
 - 22. The method according to Claim 21 wherein the potential inhibitor is designed *de novo*.
- The method of Claim 21, further comprising the steps of:

(d) contacting said potential inhibitor with KSP in the presence of a KSP binding molecule, and

(e) determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

5

10

- 24. A method for identifying a potential inhibitor of KSP function, comprising the steps of:
 - (a) generating a three-dimensional model of KSP using the relative structural coordinates as set forth in a table selected from Tables 1, 2, 3 and 4, ± a root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å;
 - (b) employing said three-dimensional model to design or select a potential inhibitor; and
- 15 (c) synthesizing or obtaining said potential inhibitor.
 - 25. The method according to Claim 24 wherein the potential inhibitor is designed *de novo*.

20

(d)

- 26. The method of Claim 24, further comprising the steps of: contacting said potential inhibitor with KSP in the presence of a KSP binding molecule, and
- (e) determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

25

27. The method of Claim 21, further comprising contacting the potential inhibitor with KSP in the presence of a KSP binding molecule, and determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

30

28. The method of Claim 21, further comprising contacting the potential inhibitor with KSP in the presence of one or two

KSP substrates selected from ATP and microtubules, and determining the effect the potential inhibitor has on KSP ATPase activity.

- 29. A potential inhibitor identified by the method of
 5 Claim 21, or a pharmaceutically acceptable salt thereof.
 - 30. A method of identifying an inhibitor compound capable of binding to kinesin spindle protein (KSP), said method comprising:
- (a) introducing protein coordinates selected from the protein coordinates

 provided in a table selected from Tables 1, 2, 3 and 4, ± a root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å, into a suitable computer program so as to define a (+)-monastrol ligand binding site conformation, wherein said program displays the three- dimensional structure of the (+)-monastrol ligand binding site;
 - (b) creating a three dimensional representation of the (+)-monastrol ligand binding site in said computer program;
 - displaying and superimposing a three dimensional representation of a test compound on the three dimensional representation of the
 (+)-monastrol ligand binding site;
 - (d) assessing whether said test compound fits spatially into the(+)-monastrol ligand binding site;

- (e) preparing said test compound that fits spatially into the (+)-monastrol ligand binding site;
- 25 (f) using said test compound in a biological assay for KSP function; and
 - (g) determining whether said test compound inhibits KSP function in said assay.
- 31. A process for identifying a potential anti-mitotic agent which upon binding to a human KSP inhibits cell proliferation, the process comprising the steps of:

(a) obtaining an X-ray diffraction pattern of a human kinesin spindle protein (KSP) crystal, wherein said KSP has been crystallized in the presence of a mixture of at least two potential ligands;

5

(d) determining whether a ligand/KSP complex is formed by comparing the electron density map calculated from the X-ray diffraction pattern of said KSP crystal to the electron density map calculated from an X-ray diffraction pattern set forth in a table selected from Table 1, 2, 3 and 4; and

10

- (c) determining whether said ligand from said ligand/KSP complex binds to the ligand binding site of said KSP according to Claim 15, such that upon binding to KSP said ligand inhibits cell proliferation.
- 32. An anti-mitotic agent identified by the process according to Claim 31, or a pharmaceutically acceptable salt thereof.

15

33. A composition comprising: (a) an anti-mitotic agent identified according to Claim 32; and (b) a pharmaceutically acceptable carrier.

20

25

30

34. A method of identifying a compound that modulates the binding of a ligand to a ligand binding site of a human KSP, said method comprising: modeling test compounds that fit spatially into a KSP ligand binding site using an atomic structural model of a KSP binding site having the relative structural coordinates as set forth in a table selected from the group consisting of Tables 1, 2, 3 and 4 for the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; screening the test compounds in an assay characterized by binding of a ligand to the ligand binding site; and identifying a test compound that modulates binding of said ligand to the KSP at its binding site.

a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to the ligand binding site of human KSP, said three-dimensional representation comprising the structural coordinates of the KSP as set forth in a table selected from Tables 1-4 or a homologue of said molecular complex, wherein said homologue comprises a binding site that has a root mean square deviation from the backbone atoms of said KSP of not more than about 2.0 Å.

5

10

15

- 36. A method for identifying an anti-mitotic agent which upon binding to a target human KSP inhibits cell proliferation, the method comprising the steps of:
 - (a) obtaining a crystal of KSP, where said KSP has been crystallized while exposed to a mixture of at least two potential ligands;
 - (b) determining whether a ligand/KSP complex is formed in said crystal; and
- (c) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.
- 37. An anti-mitotic agent identified by the methodaccording to Claim 36, or a pharmaceutically acceptable salt thereof.
 - 38. A composition comprising: (a) an anti-mitotic agent according to Claim 37; and (b) a pharmaceutically acceptable carrier.
- 39. A method for determining the three-dimensional structure of a complex of KSP with a ligand thereof, which comprises obtaining X-ray diffraction data for crystals of the complex comprising the

WO 2004/004652

5

10

20

25

30

35

ligand bound to KSP at a ligand binding site; and utilizing said data to define the three-dimensional structure of the complex.

- 40. A method for evaluating the ability of a chemical entity to associate with a ligand binding site of human KSP or with at least a portion of the site or a complex comprising the KSP binding site; said method comprising the steps of:
- (a) employing computational or experimental means to perform a fitting operation between the chemical entity and said ligand binding site of KSP having the relative structural coordinates as set forth in Table $5 \pm$ the root mean square deviation of not more than about 2.0 Å, thereby obtaining data related to said association; and
- (b) analyzing the data obtained in step (a) to determine the characteristics of the association between the chemical entity and said
 15 KSP or complex.
 - 41. A chemical entity identified by the method of Claim 37, wherein the chemical entity is capable of interfering with the *in vivo* or *in vitro* motor activity of KSP, or a pharmaceutically acceptable salt thereof.
 - 42. A composition comprising: (a) a chemical entity identified according to Claim 38; and (b) a pharmaceutically acceptable carrier.
 - 43. A method for identifying a potential inhibitor of human kinesin spindle protein (KSP), the method comprising the steps of:
 - (a) providing a three-dimensional structure of a ligand-bound KSP as defined by atomic coordinates set forth in a table selected from a group consisting of Tables 1, 2, 3 and $4 \pm$ the root mean square deviation of not more than about 2.0 Å;
 - (b) comparing the three-dimensional coordinates of the ligand when it is bound to KSP as set forth in Table 1, 2, 3 or $4 \pm$ the root mean square deviation of not more than about 2.0 Å to the three-dimensional coordinates of a compound in a database of compound structures; and

(c) selecting from said database at least one compound that is structurally similar to said ligand when it is bound to said KSP, wherein the selected compound is a potential inhibitor of said KSP.

- 5 44. The method of Claim 43, wherein the structural similarity is determined based on the root mean square deviation in the backbone atoms of the kinesin peptide and the kinesin inhibitor.
- 45. A method for identifying a potential inhibitor of a human kinesin spindle protein (KSP), the method comprising the steps of:
 - (a) providing a three-dimensional structure of said KSP as defined by atomic coordinates set forth in a table selected from Tables 1-4 ± the root mean square deviation of not more than about 2.0 Å;
- (b) employing the three-dimensional structures to design or select a potential inhibitor;
 - (c) synthesizing the potential inhibitor; and
 - (d) contacting the potential inhibitor with KSP to determine the ability of the potential inhibitor to arrest mitosis or inhibit cell proliferation.

- 46. A potential inhibitor identified by the method of Claim 45 or a pharmaceutically acceptable salt thereof.
- 47. A composition comprising: (a) the potential inhibitor identified according to Claim 46; and (b) a pharmaceutically acceptable carrier.
- 48. A method of identifying an inhibitor of KSP wherein the inhibitor binds to the ligand binding site according to Claim 13 which comprises determining the shift in the fluorescence of an amino acid residue at position 127 of KSP, wherein said amino acid residue is tryptophan.
 - 49. The method according to Claim 48 which comprises the steps of:

(a) contacting KSP with the test compound and a
 nucleotide and measuring the fluorescence of the
 mixture at the peak emission wavelength for W127 in
 KSP;

5

(b) contacting KSP with a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for W127 in KSP; and

10

(c) comparing the fluorescence of the mixture of KSP, the test compound and the nucleotide with the fluorescence of the mixture of KSP with the nucleotide alone.

50. An anti-mitotic agent characterized as:

15

(a) specifically binding to the target KSP or an analogue thereof at a ligand binding site comprising the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) according to Tables 1, 2, 3 or 4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0Å; and

20

(b) which, upon binding to said KSP or an analogue thereof specifically inhibits said KSP or analogs biological activities.

25

- 51. A method of causing the alteration of the structural conformation of a KSP protein which comprises exposing the protein to a ligand that binds to the KSP ligand binding site as set forth in Table $5 \pm$ the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å.
- 52. The method according to Claim 51 wherein the KSP protein is additionally bound to a nucleotide.

53. A method of treating or preventing hyper-proliferative diseases which comprises administering to a mammal a therapeutically effective amount of a compound that binds to the KSP ligand binding site as set forth in Table $5 \pm$ the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å.

- 54. The method according to Claim 53 which is a method of treating or preventing cancer.
- 10 55. The method according to Claim 54 which is a method of treating cancer.
- 56. An isolated and substantially pure polypeptide or a fragment thereof comprising the amino acid sequence as set forth in SEQ ID
 NO:1.
 - 57. The isolated polypeptide of Claim 56, wherein the polypeptide adopts the conformation of the ligand binding pocket as set forth in Table 5, ± the root mean square deviation of not more than about 2.0 Å.
 - 58. A variant of the isolated polypeptide according to Claim 57 having at least about 80% amino acid sequence identity with the polypeptide of Claim 57, wherein the percentage identity is determined with the algorithm Gap, BASEFIT or FASTA in the Wisconsin Genetics Software Package release 7.0, using default Gap weights.
 - 59. An active structural motif designated herein as pharmacophore model, which refers to the three-dimensional orientation of a set of features describing the physical, chemical and/or electronic environment of the active site of the human KSP, said features comprising either a hydrophobic region feature, a hydrogen bond acceptor feature and a hydrogen bond donor feature (pharmacophore model in FIG. 14A) or two hydrophobic region features and a hydrogen bond acceptor feature (pharmacophore model in FIG. 14B).

20

25

30

60. A method for screening and identifying potential KSP inhibitor compounds by evaluating the fit of the screened compounds to the pharmacophore models of claim 59.

- 5 61. The method of claim 60 wherein evaluating the fit is carried out via the use of a computer and a computer-readable medium.
- 62. A compound, comprising two hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in Figure 14B and wherein said compound inhibits the mitotic kinesin KSP; or a pharmaceutically acceptable salt thereof.
- A compound, comprising two hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in
 Figure 14B and wherein said compound fits within a ligand binding site of a kinesin spindle protein (KSP) protein, said ligand binding site comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2 Å;

or a pharmaceutically acceptable salt thereof.

- 64. The compound according to Claim 63 wherein the two hydrophobic region features are independently selected from an aryl, heteroaryl and C₃-C₇-cycloalkyl, optionally substituted.
- 25 65. The compound according to Claim 63 wherein the two hydrophobic region features are independently selected from an optionally substituted phenyl.
- 66. The compound according to Claim 63 wherein the compound has a binding affinity for KSP of about 0.1nM to about 100nM.
 - 67. A compound, comprising one hydrophobic region feature, a hydrogen bond donor feature and a hydrogen bond acceptor feature, wherein said

5

10

20

features are oriented as illustrated in Figure 14A and wherein said compound inhibits the mitotic kinesin KSP;

or a pharmaceutically acceptable salt thereof.

68. A compound, comprising one hydrophobic region feature, a hydrogen bond donor feature and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in Figure 14A and wherein said compound fits within a ligand binding site of a kinesin spindle protein (KSP) protein, said ligand binding site comprising the relative structural coordinates set forth in Table $5 \pm$ the root mean square deviation from the backbone atoms of said amino acids of not more than about 2 Å;

or a pharmaceutically acceptable salt thereof.

- 69. The compound according to Claim 68 wherein the hydrophobic region feature is selected from an aryl, heteroaryl and C₃-C₇-cycloalkyl, optionally substituted.
 - 70. The compound according to Claim 68 wherein the hydrophobic region feature is selected from an optionally substituted phenyl.
 - 71. The compound according to Claim 68 wherein the compound has a binding affinity for KSP of about 0.1nM to about 100nM.
- 72. The compound according to Claim 68 wherein the compound does not comprise a 2-thioxo-1,2,3,4-tetrahydopyrimidine moiety, a dihydropyrimidine moiety or a 5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]-pyrido[3.4-b]indole-1,3(2H)-dione moiety.
- 73. A compound, comprising three hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are spatially oriented as illustrated in Figure 16 and have the distances in Å between the features as follows

	1	2	3	4
1	_			
2	5.1±0.6	-		
3	8.5±0.7	6.9±0.7	-	
4	3.7±0.5	5.8±0.6	5.7±0.7	-

and wherein said compound inhibits the mitotic kinesin KSP; or a pharmaceutically acceptable salt thereof.

The compound according to Claim 73 wherein the compound does not comprise a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety.

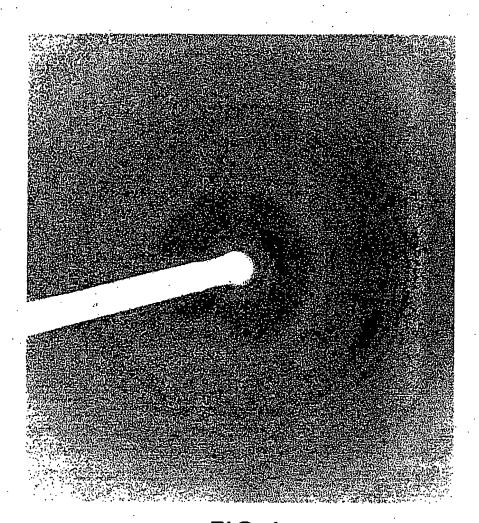


FIG.1

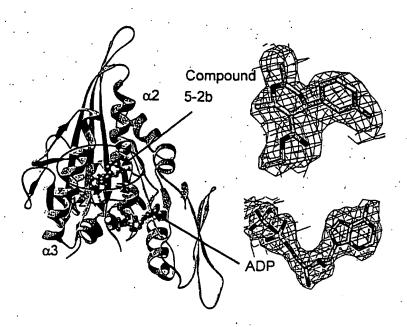


FIG.2

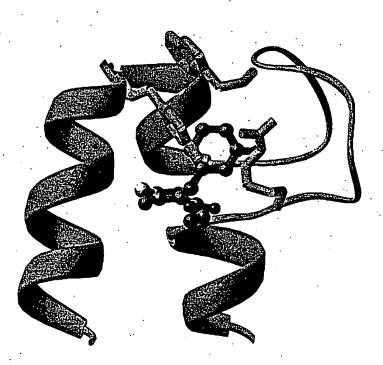


FIG.3

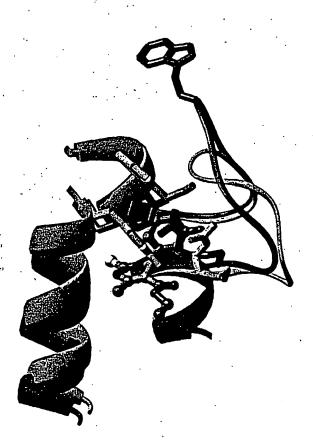


FIG.4

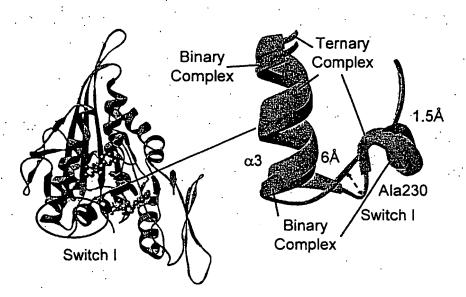


FIG.5

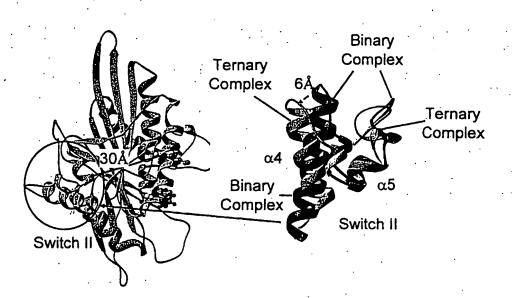


FIG.6

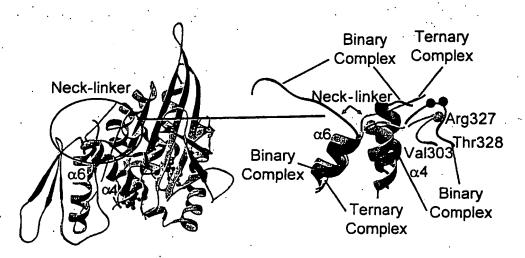


FIG.7

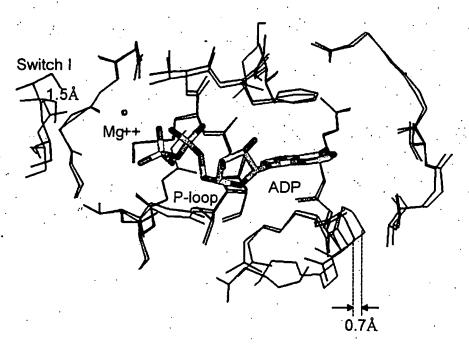


FIG.8

.Seq. ID #1

MASQPNSSAK KKEEKGKNIQ VVVRCRPFNL AERKASAHSI VECDPVRKEV SVRTGGLADK SSRKTYTFDM VFGASTKQID VYRSVVCPIL DEVIMGYNCT IFAYGQTGTG KTFTMEGERS PNEEYTWEED PLAGIIPRTL HQIFEKLTDN GTEFSVKVSL LEIYNEELFD LLNPSSDVSE RLQMFDDPRN KRGVIIKGLE EITVHNKDEV YQILEKGAAK RTTAATLMNA YSSRSHSVFS VTIHMKETTI DGEELVKIGK LNLVDLAGSE NIGRSGAVDK RAREAGNINQ SLLTLGRVIT ALVERTPHVP YRESKLTRIL QDSLGGRTRT SIIATISPAS LNLEETLSTL EYAHRAKNIL NKPEVNQK

FIG.9

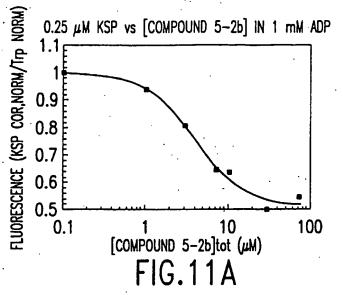
115(M), 116(E), 117(G), 118(E), 119(R);

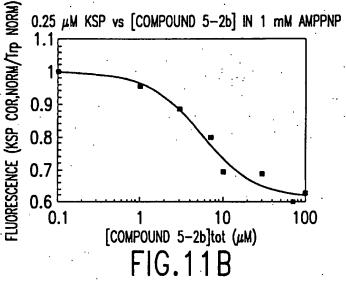
127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P);

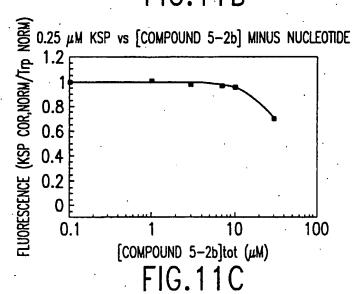
160(L); and

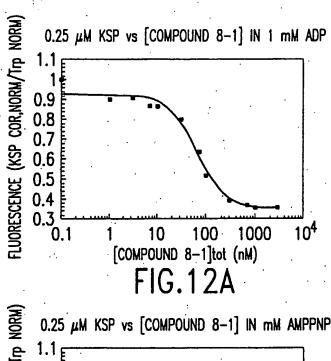
211(Y), 214(L), 215(E), 217(G), 218(A), 221(R), 239(F).

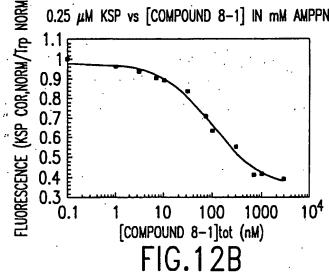
FIG. 10

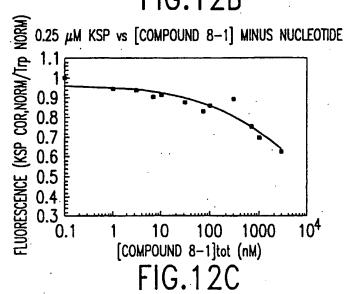




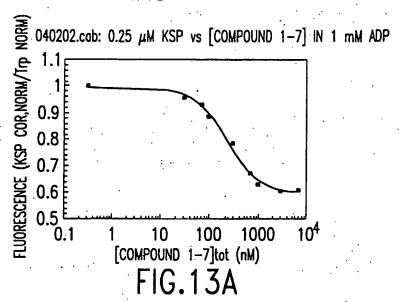


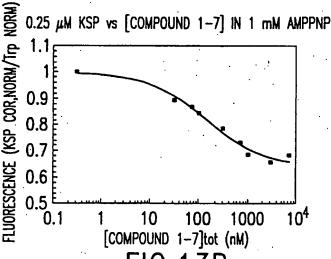


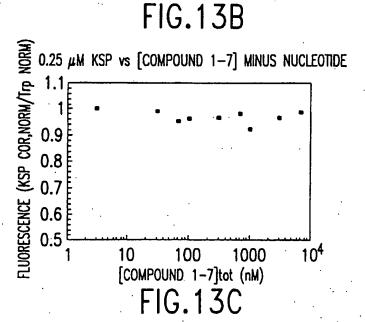












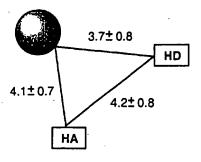


FIG. 14A

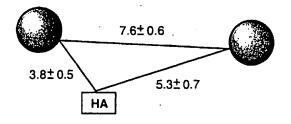


FIG. 14B

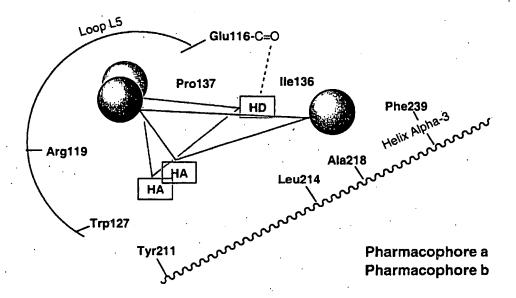


FIG. 15

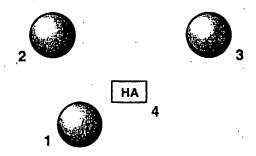


FIG. 16

SEQUENCE LISTING

<110> Merck & Co., Inc. Buser-Doepner, Carolyn A. Coleman, Paul J. Cox, Christopher D. Fraley, Mark E. Garbaccio, Robert M. Hartman, George D. Heimbrook, David C. Huber, Hans E. Kuo, Lawrence C. Sardana, Vinod V. Torrent, Maricel Youwei, Yan

<120> MITOTIC KINESIN BINDING SITE

<130> 21125Y

<150> 60/394,313

<151> 2002-07-08

<160> 1

<170> FastSEQ for Windows Version 4.0

<210> 1

<211> 368

<212> PRT

<213> human

<400> 1 Met Ala Ser Gln Pro Asn Ser Ser Ala Lys Lys Lys Glu Glu Lys Gly 10 15 Lys Asn Ile Gln Val Val Val Arg Cys Arg Pro Phe Asn Leu Ala Glu 20 25 Arg Lys Ala Ser Ala His Ser Ile Val Glu Cys Asp Pro Val Arg Lys 35 40 Glu Val Ser Val Arg Thr Gly Gly Leu Ala Asp Lys Ser Ser Arg Lys 50 55 60 Thr Tyr Thr Phe Asp Met Val Phe Gly Ala Ser Thr Lys Gln Ile Asp 65 70 75 Val Tyr Arg Ser Val Val Cys Pro Ile Leu Asp Glu Val Ile Met Gly 85 90 Tyr Asn Cys Thr Ile Phe Ala Tyr Gly Gln Thr Gly Thr Gly Lys Thr 100 105 110 Phe Thr Met Glu Gly Glu Arg Ser Pro Asn Glu Glu Tyr Thr Trp Glu 115 120 125 Glu Asp Pro Leu Ala Gly Ile Ile Pro Arg Thr Leu His Gln Ile Phe 130 135 Glu Lys Leu Thr Asp Asn Gly Thr Glu Phe Ser Val Lys Val Ser Leu 145 150 155 Leu Glu Ile Tyr Asn Glu Glu Leu Phe Asp Leu Leu Asn Pro Ser Ser

Asp Val Ser Glu Arg Leu Gln Met Phe Asp Asp Pro Arg Asn Lys Arg

170

			180					185					190		
Gly	Val	Ile 195	Ile	Lys	Gly	Leu		Glu		Thr	Val	His 205	Asn	Lys	Asp
Glu	Val 210	Tyr	Gln	Ile	Leu	Glu 215	Lys	Gly	Ala	Ala	Lys 220		Thr	Thr	Ala
Ala 225	Thr	Leu	Met	Asn	Ala 230	Tyr	Ser	Ser	Arg	Ser 235	His	Ser	Val	Phe	Ser 240
				245					250				Glu	255	Val
			260					265					Glu 270		
		275					280					285	Gly		
	290					295					300		Leu		
305					310					315			Arg		320
				325					330				Ala	335	
			340				•	345					Leu 350		
Ala	His	Arg 355	Ala	Lys	Asn	Ile	Leu 360	Asn	Lys	Pro	Glu	Val 365	Asn	Gln	Lys